



Full wwPDB EM Validation Report ⓘ

Aug 10, 2022 – 12:05 am BST

PDB ID : 7PNK
EMDB ID : EMD-13548
Title : Unstacked compact Dunaliella PSII
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on : 2021-09-07
Resolution : 3.61 Å(reported)
Based on initial model : 6KAC

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

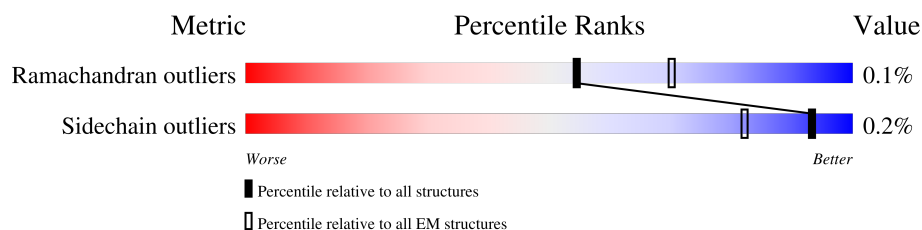
EMDB validation analysis : 0.0.1.dev8
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

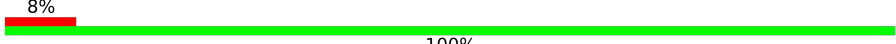
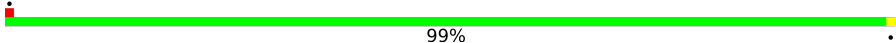
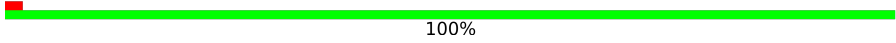
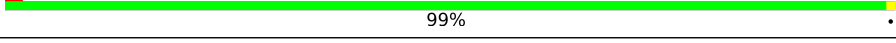
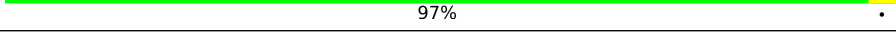
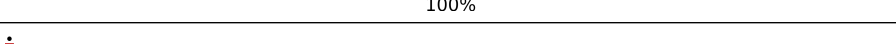
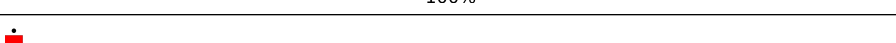


The reported resolution of this entry is 3.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



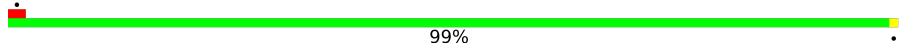
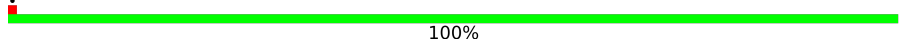
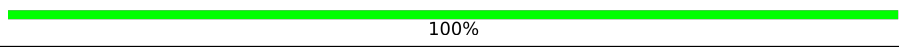
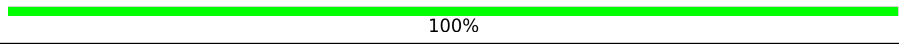
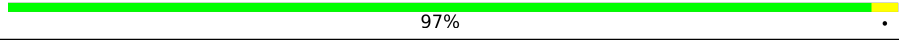
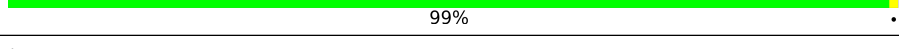
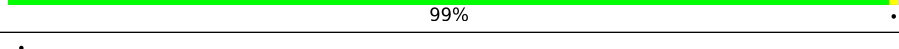
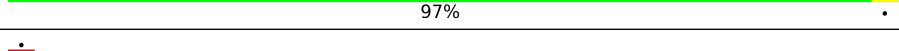
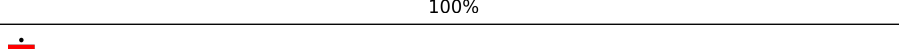
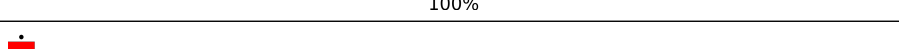
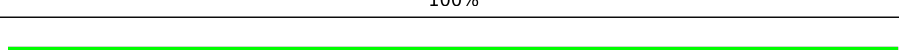
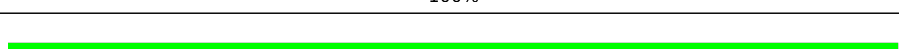
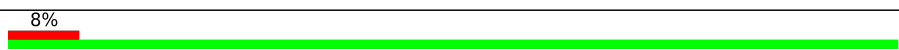
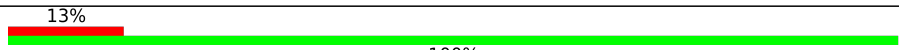
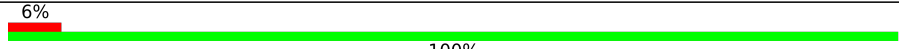

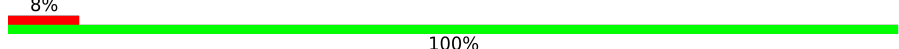
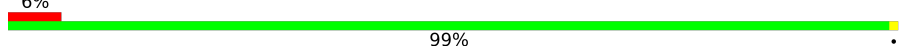
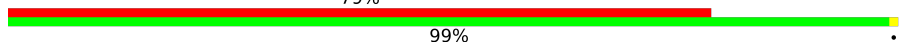
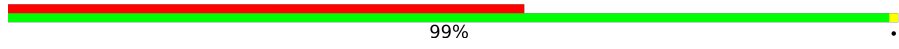
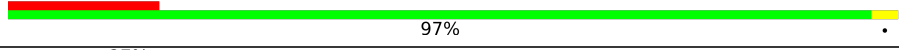
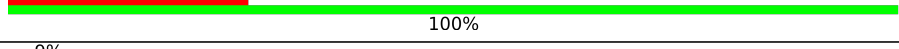
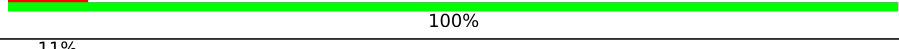
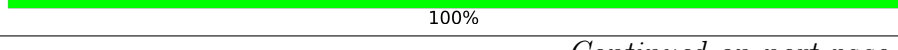

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	 8% 100%
1	a	336	 99%
2	B	484	 100%
2	b	484	 99%
3	V	32	 97%
3	v	32	 100%
4	C	449	 100%
4	c	449	 100%
5	D	348	 100%

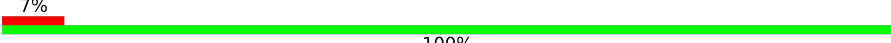
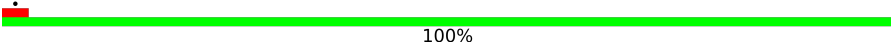
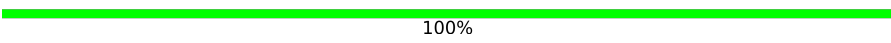
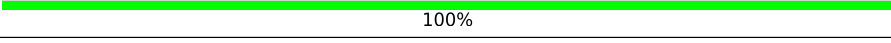
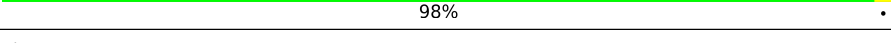
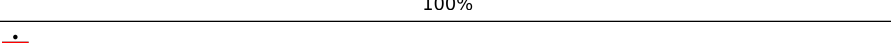
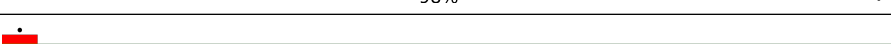



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Mol	Chain	Length	Quality of chain
5	d	348	 99%
6	E	76	 100%
6	e	76	 100%
7	F	31	 100%
7	f	31	 97%
8	H	67	 99%
8	h	67	 99%
9	I	35	 97%
9	i	35	 100%
10	J	36	 100%
10	j	36	 100%
11	K	37	 100%
11	k	37	 100%
12	L	38	 8%100%
12	l	38	 13%100%
13	M	31	 6%100%
13	m	31	 16%100%
14	O	238	 8%100%
14	o	238	 6%99%
15	P	187	 79%99%
15	p	187	 58%99%
16	T	30	 17%97%
16	t	30	 27%100%
17	W	44	 9%100%
17	w	44	 11%100%

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Mol	Chain	Length	Quality of chain
18	X	30	 100%
18	x	30	 100%
19	Z	61	 100%
19	z	61	 100%
20	N	222	 98%
21	G	221	 100%
22	S	243	 98%
23	Y	222	 100%
24	U	27	 100%
24	u	27	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	A	405	X	-	-	-
28	CLA	A	406	X	-	-	-
28	CLA	A	407	X	-	-	-
28	CLA	A	410	X	-	-	-
28	CLA	B	602	X	-	-	-
28	CLA	B	603	X	-	-	-
28	CLA	B	604	X	-	-	-
28	CLA	B	605	X	-	-	-
28	CLA	B	606	X	-	-	-
28	CLA	B	607	X	-	-	-
28	CLA	B	608	X	-	-	-
28	CLA	B	609	X	-	-	-
28	CLA	B	610	X	-	-	-
28	CLA	B	611	X	-	-	-
28	CLA	B	612	X	-	-	-
28	CLA	B	613	X	-	-	-
28	CLA	B	614	X	-	-	-
28	CLA	B	615	X	-	-	-
28	CLA	B	616	X	-	-	-
28	CLA	B	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	C	501	X	-	-	-
28	CLA	C	502	X	-	-	-
28	CLA	C	503	X	-	-	-
28	CLA	C	504	X	-	-	-
28	CLA	C	505	X	-	-	-
28	CLA	C	506	X	-	-	-
28	CLA	C	507	X	-	-	-
28	CLA	C	508	X	-	-	-
28	CLA	C	509	X	-	-	-
28	CLA	C	510	X	-	-	-
28	CLA	C	511	X	-	-	-
28	CLA	C	512	X	-	-	-
28	CLA	C	513	X	-	-	-
28	CLA	D	402	X	-	-	-
28	CLA	D	403	X	-	-	-
28	CLA	G	602	X	-	-	-
28	CLA	G	603	X	-	-	-
28	CLA	G	604	X	-	-	-
28	CLA	G	610	X	-	-	-
28	CLA	G	611	X	-	-	-
28	CLA	G	612	X	-	-	-
28	CLA	G	613	X	-	-	-
28	CLA	G	614	X	-	-	-
28	CLA	N	602	X	-	-	-
28	CLA	N	603	X	-	-	-
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28	CLA	S	602	X	-	-	-
28	CLA	S	603	X	-	-	-
28	CLA	S	604	X	-	-	-
28	CLA	S	605	X	-	-	-
28	CLA	S	609	X	-	-	-
28	CLA	S	610	X	-	-	-
28	CLA	S	611	X	-	-	-
28	CLA	S	612	X	-	-	-
28	CLA	S	613	X	-	-	-
28	CLA	S	614	X	-	-	-
28	CLA	S	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	Y	602	X	-	-	-
28	CLA	Y	603	X	-	-	-
28	CLA	Y	604	X	-	-	-
28	CLA	Y	608	X	-	-	-
28	CLA	Y	610	X	-	-	-
28	CLA	Y	611	X	-	-	-
28	CLA	Y	612	X	-	-	-
28	CLA	Y	613	X	-	-	-
28	CLA	Y	614	X	-	-	-
28	CLA	a	405	X	-	-	-
28	CLA	a	406	X	-	-	-
28	CLA	a	407	X	-	-	-
28	CLA	a	410	X	-	-	-
28	CLA	b	602	X	-	-	-
28	CLA	b	603	X	-	-	-
28	CLA	b	604	X	-	-	-
28	CLA	b	605	X	-	-	-
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28	CLA	c	503	X	-	-	-
28	CLA	c	504	X	-	-	-
28	CLA	c	505	X	-	-	-
28	CLA	c	506	X	-	-	-
28	CLA	c	507	X	-	-	-
28	CLA	c	508	X	-	-	-
28	CLA	c	509	X	-	-	-
28	CLA	c	510	X	-	-	-
28	CLA	c	511	X	-	-	-
28	CLA	c	512	X	-	-	-
28	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	d	402	X	-	-	-
28	CLA	d	403	X	-	-	-
34	C7Z	B	620	X	-	-	-
34	C7Z	b	620	X	-	-	-
39	LMK	C	527	X	-	-	-
39	LMK	c	527	X	-	-	-
43	RRX	H	101	X	-	-	-
43	RRX	h	101	X	-	-	-
46	CHL	G	601	X	-	-	-
46	CHL	G	605	X	-	-	-
46	CHL	G	606	X	-	-	-
46	CHL	G	607	X	-	-	-
46	CHL	G	608	X	-	-	-
46	CHL	G	609	X	-	-	-
46	CHL	N	601	X	-	-	-
46	CHL	N	605	X	-	-	-
46	CHL	N	606	X	-	-	-
46	CHL	N	607	X	-	-	-
46	CHL	N	608	X	-	-	-
46	CHL	N	609	X	-	-	-
46	CHL	S	601	X	-	-	-
46	CHL	S	606	X	-	-	-
46	CHL	S	607	X	-	-	-
46	CHL	S	608	X	-	-	-
46	CHL	Y	601	X	-	-	-
46	CHL	Y	605	X	-	-	-
46	CHL	Y	606	X	-	-	-
46	CHL	Y	607	X	-	-	-
46	CHL	Y	609	X	-	-	-
48	XAT	G	622	X	-	-	-
48	XAT	N	622	X	-	-	-

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 60673 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		
2	b	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			227	152	37	38		
3	v	32	Total	C	N	O	0	0
			227	152	37	38		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	76	Total	C	N	O	S	0	0
			621	404	102	115			
6	e	76	Total	C	N	O	S	0	0
			621	404	102	115			

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

- Molecule 9 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

- Molecule 10 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			266	183	40	43		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	36	Total	C	N	O	0	0
			266	183	40	43		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	7	ILE	THR	conflict	UNP A0A1C8XRM8
J	42	LEU	GLN	conflict	UNP A0A1C8XRM8
j	7	ILE	THR	conflict	UNP A0A1C8XRM8
j	42	LEU	GLN	conflict	UNP A0A1C8XRM8

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	207	43	47		
11	k	37	Total	C	N	O	0	0
			297	207	43	47		

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	l	38	Total	C	N	O	S	0	0
			313	209	51	52	1		

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			234	159	33	42		
13	m	31	Total	C	N	O	0	0
			234	159	33	42		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	9	THR	ILE	conflict	UNP D0FXZ3
m	9	THR	ILE	conflict	UNP D0FXZ3

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1822	1153	296	367	6		
14	o	238	Total	C	N	O	S	0	0
			1822	1153	296	367	6		

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	30	Total	C	N	O		0	0
			201	132	32	37			
18	x	30	Total	C	N	O		0	0
			201	132	32	37			

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called Chlorophyll a-b binding protein of LHCII type I, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	180	ALA	PRO	conflict	UNP A1XKU7

- Molecule 22 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

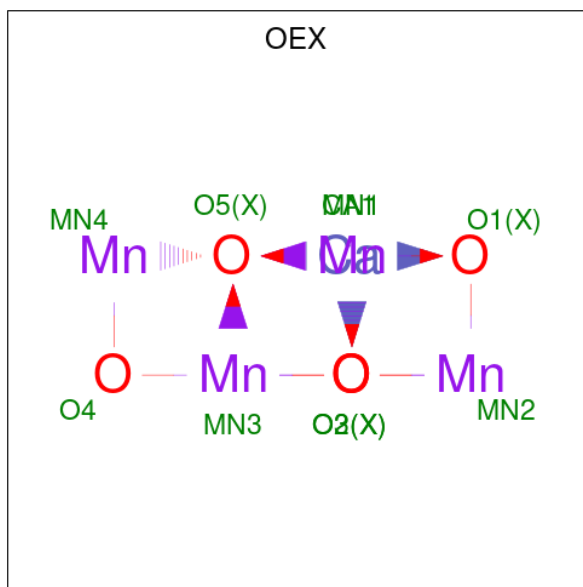
- Molecule 23 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	222	Total	C	N	O	S	0	0
			1670	1083	272	312	3		

- Molecule 24 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
24	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

- Molecule 25 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
25	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

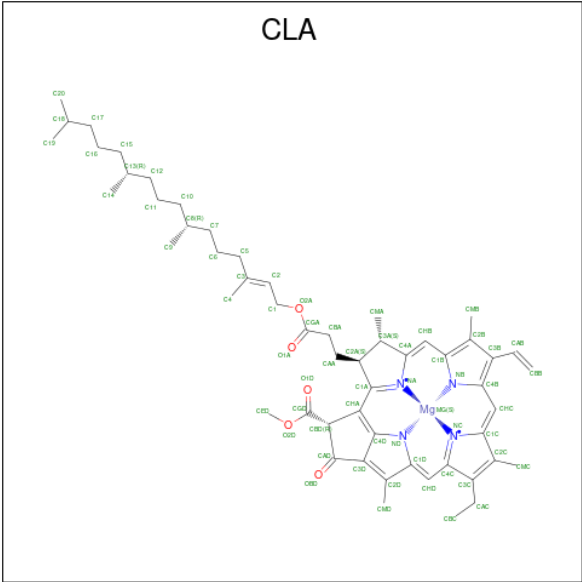
- Molecule 26 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	Fe	0
			1	1	
26	a	1	Total	Fe	0
			1	1	

- Molecule 27 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
27	A	2	Total	Cl	0
			2	2	
27	a	2	Total	Cl	0
			2	2	

- Molecule 28 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
28	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
28	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
28	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
28	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	

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Mol	Chain	Residues	Atoms					AltConf
28	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
28	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
28	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
28	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
28	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
28	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
28	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
28	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
28	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
28	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
28	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
28	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
28	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
28	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
28	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
28	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
28	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
28	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
28	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
28	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
28	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
28	S	1	Total 625	C 515	Mg 11	N 44	O 55	0

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Mol	Chain	Residues	Atoms					AltConf
28	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
28	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
28	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
28	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
28	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
28	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
28	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
28	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
28	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
28	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
28	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
28	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
28	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
28	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
28	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
28	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
28	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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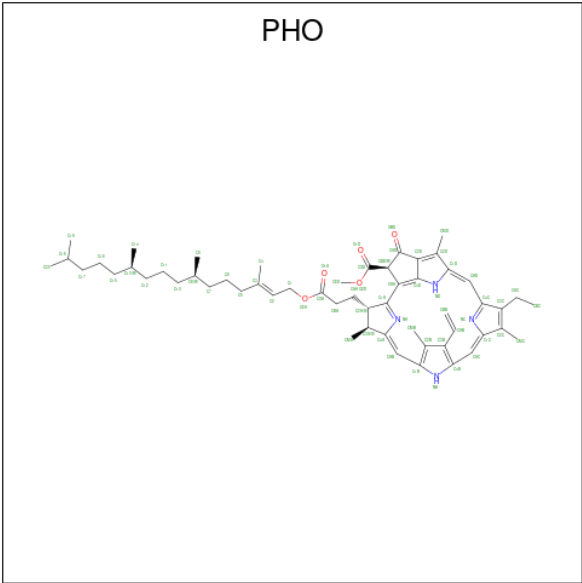
Mol	Chain	Residues	Atoms					AltConf
28	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
28	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
28	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
28	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
28	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	

- Molecule 29 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



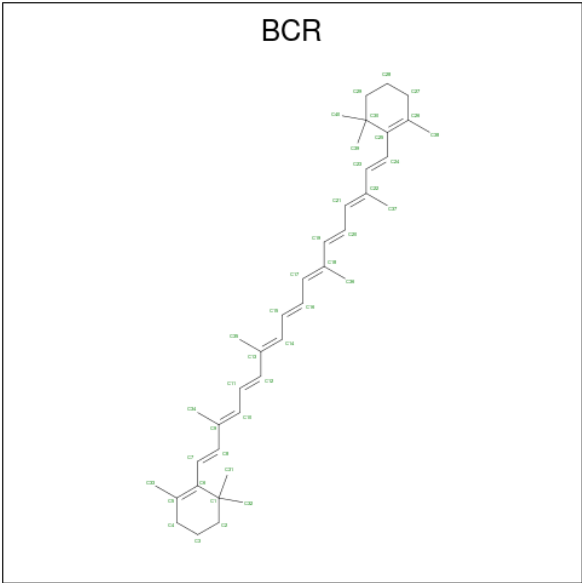
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	N	O	0
			128	110	8	10	
29	A	1	Total	C	N	O	0
			128	110	8	10	
29	a	1	Total	C	N	O	0
			128	110	8	10	

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Mol	Chain	Residues	Atoms				AltConf
29	a	1	Total	C	N	O	0
			128	110	8	10	

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



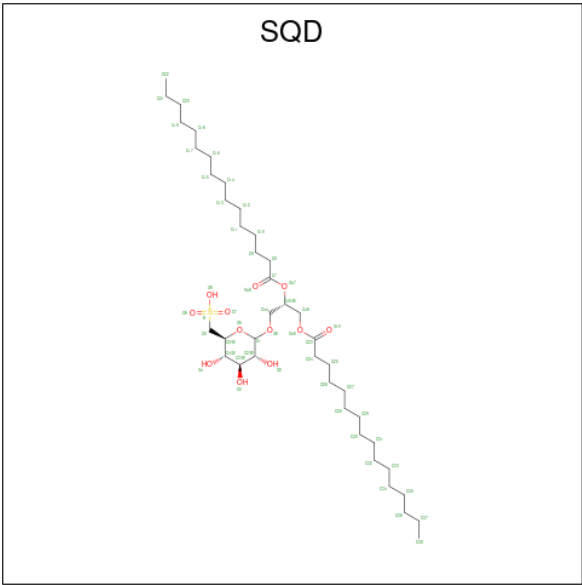
Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	C	0
			40	40	
30	B	1	Total	C	0
			80	80	
30	B	1	Total	C	0
			80	80	
30	C	1	Total	C	0
			160	160	
30	C	1	Total	C	0
			160	160	
30	C	1	Total	C	0
			160	160	
30	C	1	Total	C	0
			160	160	
30	D	1	Total	C	0
			40	40	
30	a	1	Total	C	0
			40	40	
30	b	1	Total	C	0
			80	80	

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Mol	Chain	Residues	Atoms		AltConf
30	b	1	Total	C	0
			80	80	
30	c	1	Total	C	0
			160	160	
30	c	1	Total	C	0
			160	160	
30	c	1	Total	C	0
			160	160	
30	c	1	Total	C	0
			160	160	
30	d	1	Total	C	0
			40	40	

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



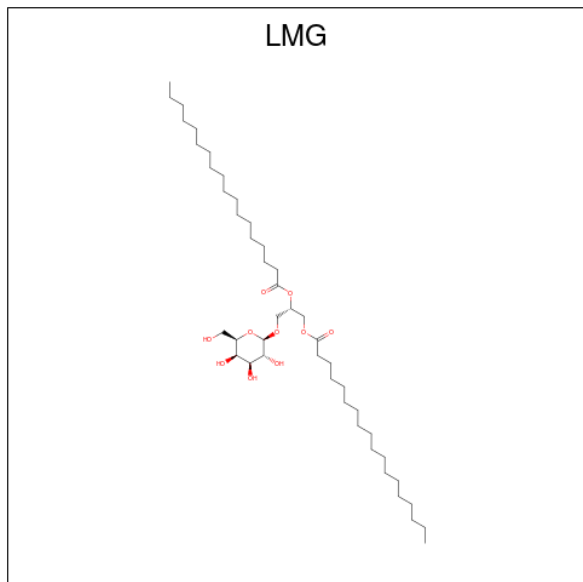
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	S	0
			51	38	12	1	
31	B	1	Total	C	O	S	0
			96	70	24	2	
31	B	1	Total	C	O	S	0
			96	70	24	2	
31	C	1	Total	C	O	S	0
			54	41	12	1	
31	M	1	Total	C	O	S	0
			42	29	12	1	

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Mol	Chain	Residues	Atoms				AltConf
31	a	1	Total	C	O	S	0
			51	38	12	1	
31	b	1	Total	C	O	S	0
			96	70	24	2	
31	b	1	Total	C	O	S	0
			96	70	24	2	
31	c	1	Total	C	O	S	0
			54	41	12	1	
31	m	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



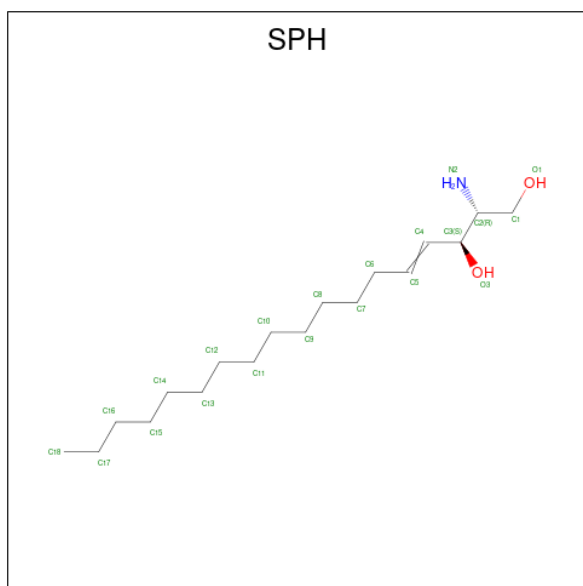
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O		0
			48	38	10		
32	B	1	Total	C	O		0
			44	34	10		
32	C	1	Total	C	O		0
			106	86	20		
32	C	1	Total	C	O		0
			106	86	20		
32	D	1	Total	C	O		0
			46	36	10		
32	H	1	Total	C	O		0
			48	38	10		

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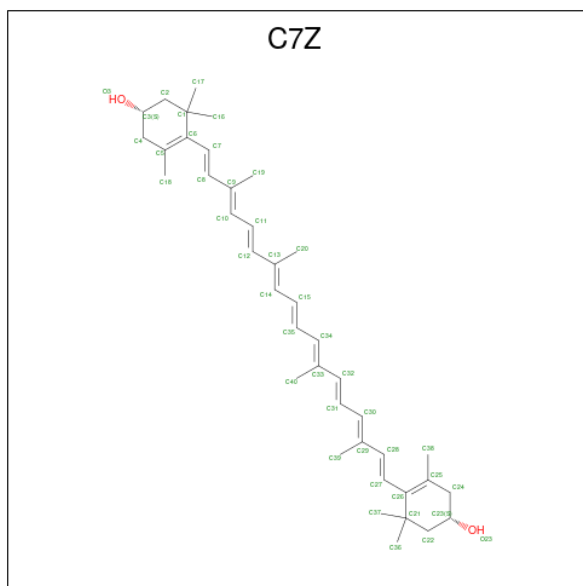
Mol	Chain	Residues	Atoms			AltConf
32	W	1	Total	C	O	0
			39	29	10	
32	a	1	Total	C	O	0
			48	38	10	
32	b	1	Total	C	O	0
			44	34	10	
32	c	1	Total	C	O	0
			106	86	20	
32	c	1	Total	C	O	0
			106	86	20	
32	d	1	Total	C	O	0
			46	36	10	
32	h	1	Total	C	O	0
			48	38	10	
32	w	1	Total	C	O	0
			39	29	10	

- Molecule 33 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



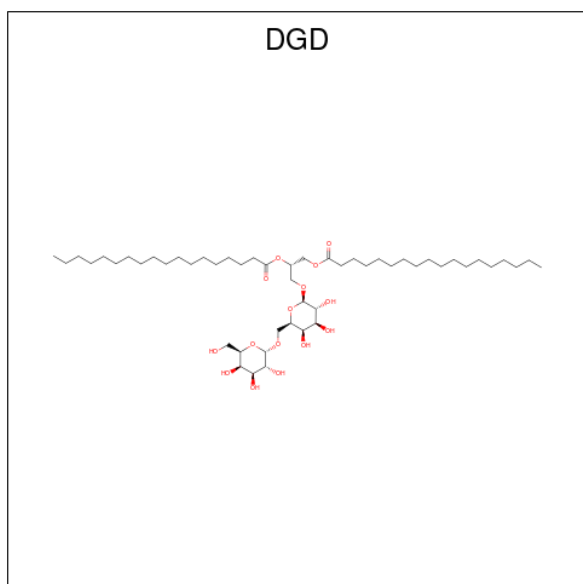
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	N	O	0
			21	18	1	2	
33	Y	1	Total	C	N	O	0
			21	18	1	2	
33	a	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 34 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: $C_{40}H_{56}O_2$).



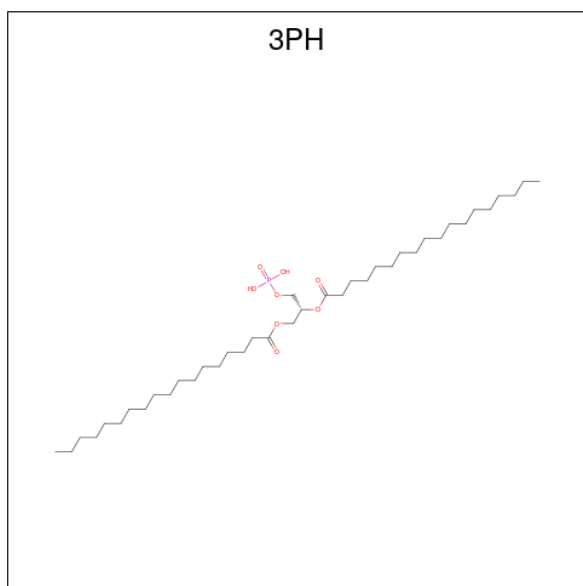
Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			42	40	2	
34	b	1	Total	C	O	0
			42	40	2	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			43	28	15	
35	C	1	Total	C	O	0
			176	131	45	
35	C	1	Total	C	O	0
			176	131	45	
35	C	1	Total	C	O	0
			176	131	45	
35	b	1	Total	C	O	0
			43	28	15	
35	c	1	Total	C	O	0
			176	131	45	
35	c	1	Total	C	O	0
			176	131	45	
35	c	1	Total	C	O	0
			176	131	45	

- Molecule 36 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



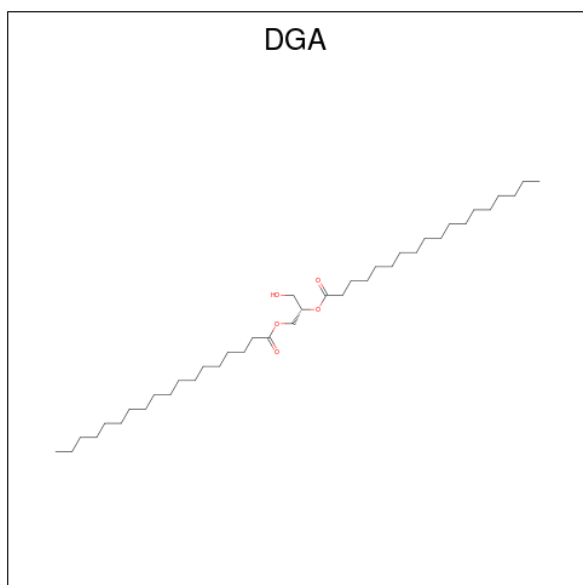
Mol	Chain	Residues	Atoms				AltConf
36	B	1	Total	C	O	P	0
			48	39	8	1	
36	T	1	Total	C	O	P	0
			48	39	8	1	
36	S	1	Total	C	O	P	0
			48	39	8	1	

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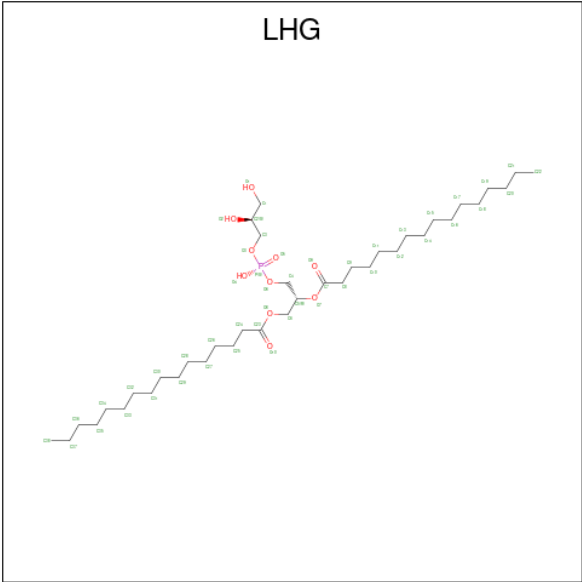
Mol	Chain	Residues	Atoms				AltConf
36	b	1	Total	C	O	P	0
			48	39	8	1	
36	t	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 37 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



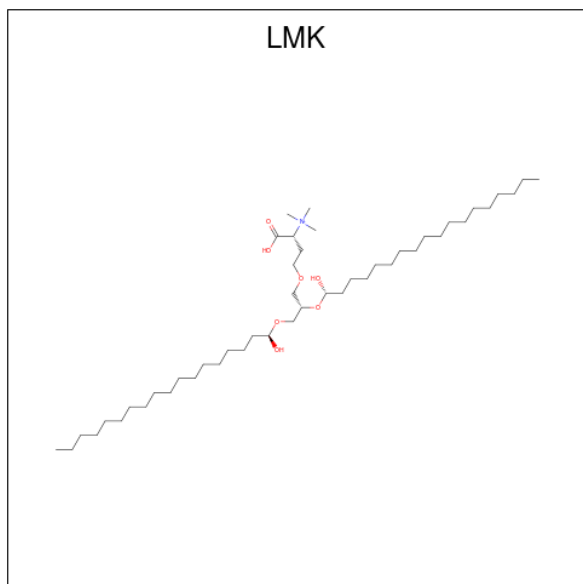
Mol	Chain	Residues	Atoms				AltConf
37	B	1	Total	C	O		0
			44	39	5		
37	C	1	Total	C	O		0
			44	39	5		
37	J	1	Total	C	O		0
			29	24	5		
37	b	1	Total	C	O		0
			44	39	5		
37	c	1	Total	C	O		0
			44	39	5		
37	j	1	Total	C	O		0
			29	24	5		

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



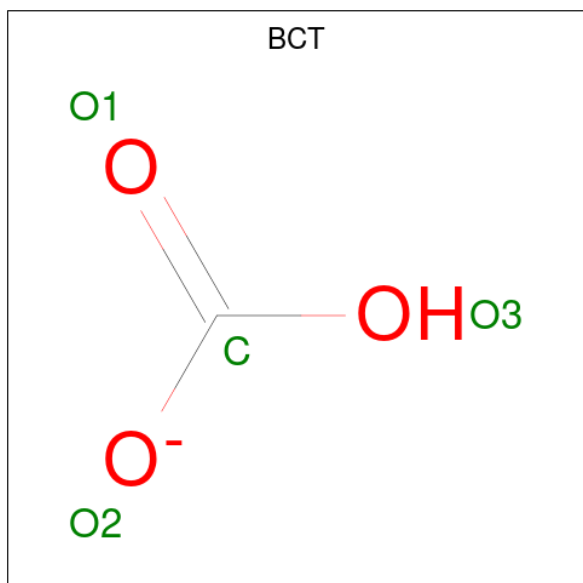
Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total	C	O	P	0
			47	36	10	1	
38	D	1	Total	C	O	P	0
			132	99	30	3	
38	D	1	Total	C	O	P	0
			132	99	30	3	
38	D	1	Total	C	O	P	0
			132	99	30	3	
38	L	1	Total	C	O	P	0
			49	38	10	1	
38	N	1	Total	C	O	P	0
			49	38	10	1	
38	G	1	Total	C	O	P	0
			49	38	10	1	
38	S	1	Total	C	O	P	0
			45	34	10	1	
38	Y	1	Total	C	O	P	0
			49	38	10	1	
38	c	1	Total	C	O	P	0
			47	36	10	1	
38	d	1	Total	C	O	P	0
			132	99	30	3	
38	d	1	Total	C	O	P	0
			132	99	30	3	
38	d	1	Total	C	O	P	0
			132	99	30	3	
38	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 39 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxido-nyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (three-letter code: LMK) (formula: $C_{46}H_{94}NO_7$).



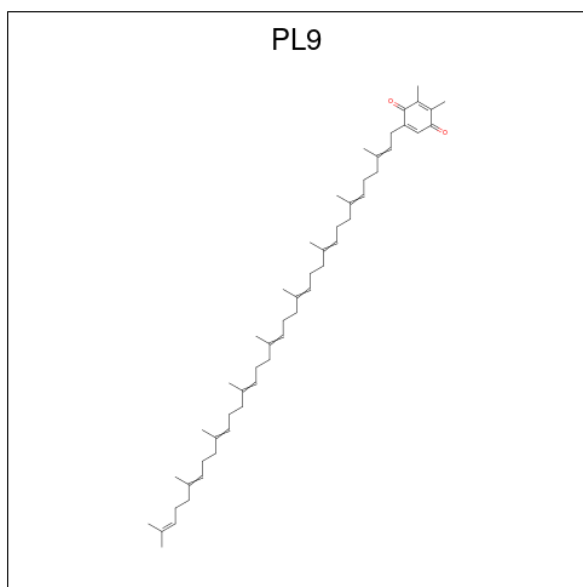
Mol	Chain	Residues	Atoms				AltConf
39	C	1	Total	C	N	O	0
			40	32	1	7	
39	c	1	Total	C	N	O	0
			40	32	1	7	

- Molecule 40 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



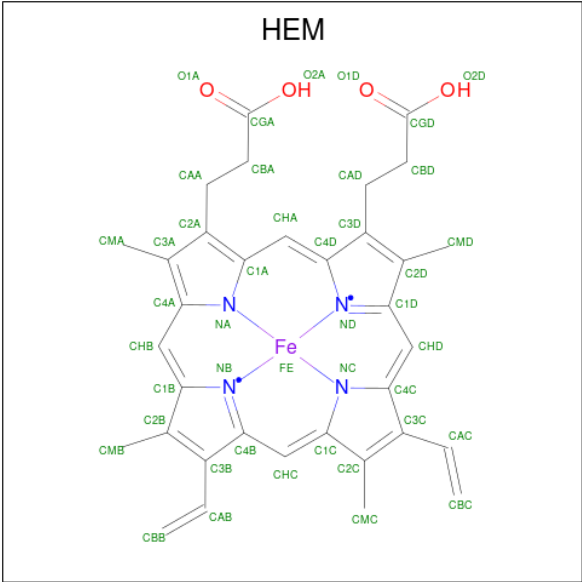
Mol	Chain	Residues	Atoms			AltConf
40	D	1	Total	C	O	0
			4	1	3	
40	d	1	Total	C	O	0
			4	1	3	

- Molecule 41 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



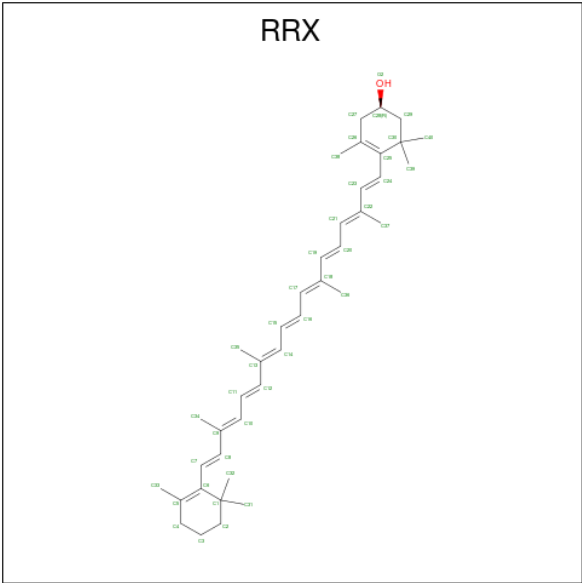
Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			55	53	2	
41	d	1	Total	C	O	0
			55	53	2	

- Molecule 42 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



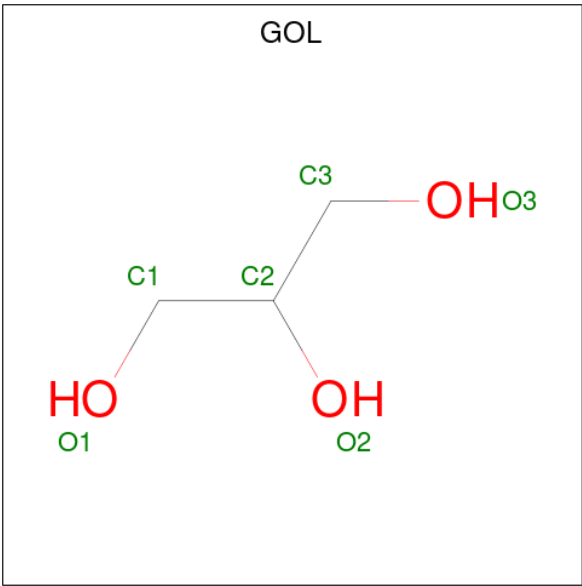
Mol	Chain	Residues	Atoms					AltConf
42	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
42	f	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 43 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C₄₀H₅₆O).



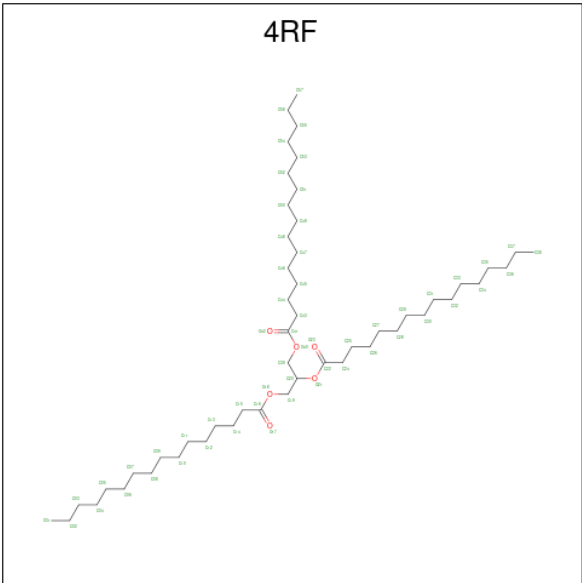
Mol	Chain	Residues	Atoms			AltConf
43	H	1	Total	C	O	0
			41	40	1	
43	h	1	Total	C	O	0
			41	40	1	

- Molecule 44 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			AltConf
44	I	1	Total	C	O	0
			6	3	3	

- Molecule 45 is Tripalmitoylglycerol (three-letter code: 4RF) (formula: C₅₁H₉₈O₆).



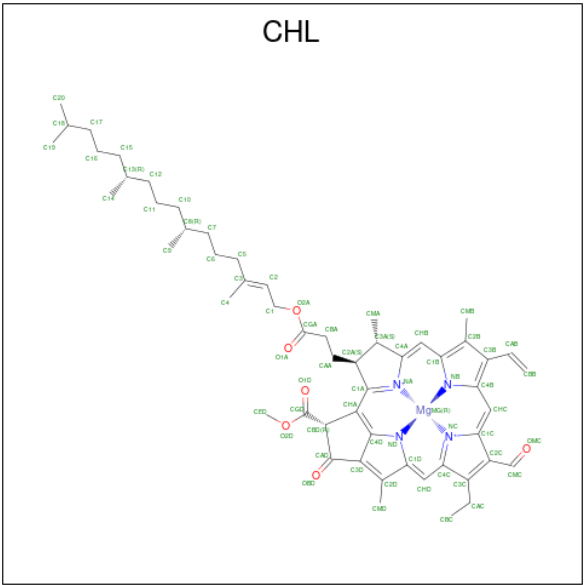
Mol	Chain	Residues	Atoms			AltConf
45	I	1	Total	C	O	0
			57	51	6	
45	K	1	Total	C	O	0
			57	51	6	

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Mol	Chain	Residues	Atoms			AltConf
45	i	1	Total	C	O	0
			57	51	6	
45	k	1	Total	C	O	0
			57	51	6	

- Molecule 46 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



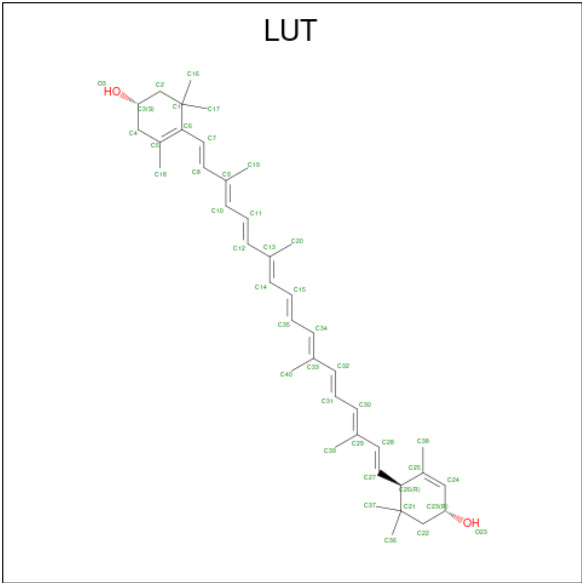
Mol	Chain	Residues	Atoms					AltConf
46	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
46	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
46	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
46	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
46	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
46	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
46	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
46	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
46	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	

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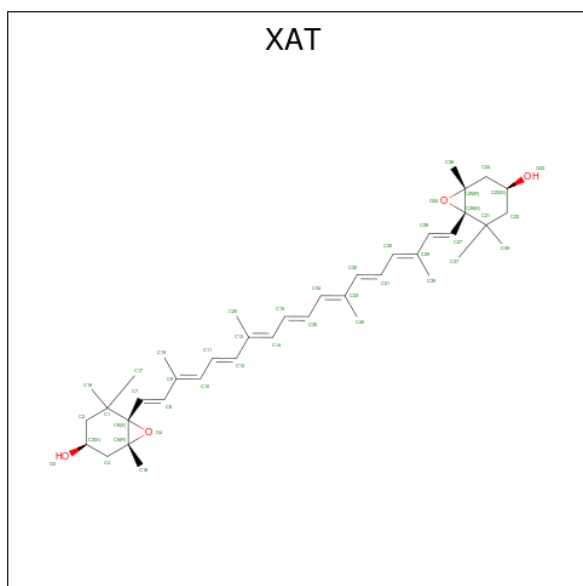
Mol	Chain	Residues	Atoms					AltConf
46	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
46	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
46	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
46	S	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
46	S	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
46	S	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
46	S	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
46	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
46	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
46	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
46	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
46	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	

- Molecule 47 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



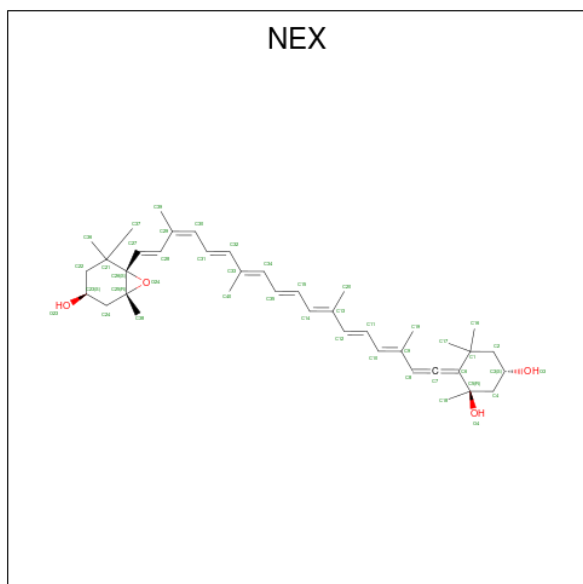
Mol	Chain	Residues	Atoms			AltConf
47	N	1	Total	C	O	0
			84	80	4	
47	N	1	Total	C	O	0
			84	80	4	
47	G	1	Total	C	O	0
			84	80	4	
47	G	1	Total	C	O	0
			84	80	4	
47	S	1	Total	C	O	0
			84	80	4	
47	S	1	Total	C	O	0
			84	80	4	
47	Y	1	Total	C	O	0
			84	80	4	
47	Y	1	Total	C	O	0
			84	80	4	

- Molecule 48 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



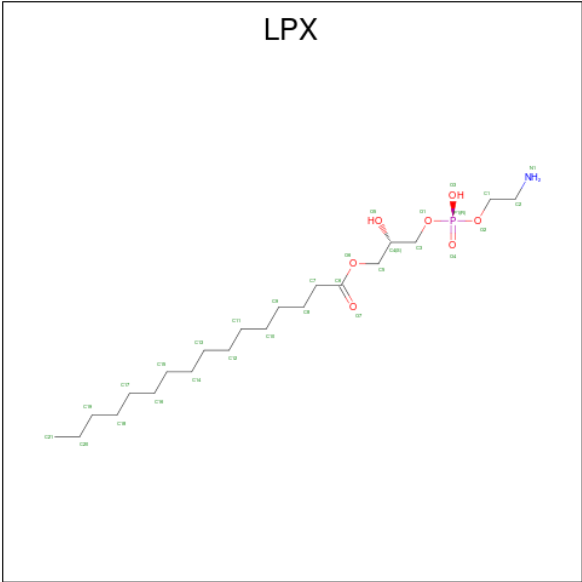
Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			44	40	4	
48	G	1	Total	C	O	0
			44	40	4	
48	Y	1	Total	C	O	0
			44	40	4	

- Molecule 49 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



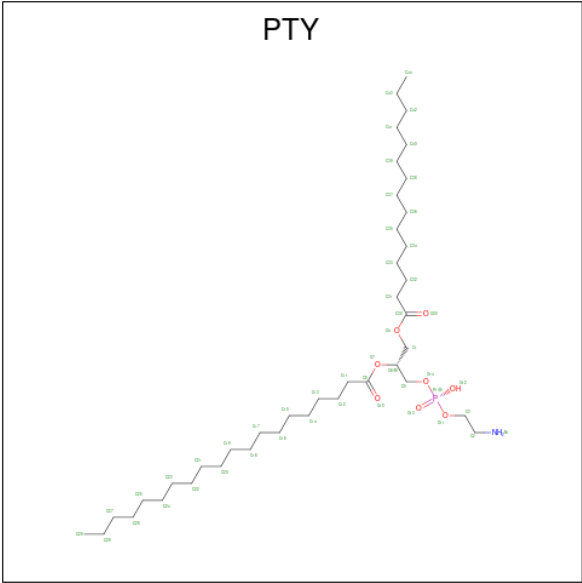
Mol	Chain	Residues	Atoms			AltConf
49	N	1	Total	C	O	0
			44	40	4	
49	G	1	Total	C	O	0
			44	40	4	
49	S	1	Total	C	O	0
			44	40	4	
49	Y	1	Total	C	O	0
			44	40	4	

- Molecule 50 is (2S)-3-[[[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-hydroxypropyl]hexadecanoate (three-letter code: LPX) (formula: C₂₁H₄₄NO₇P).



Mol	Chain	Residues	Atoms					AltConf
50	S	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 51 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C₄₀H₈₀NO₈P).

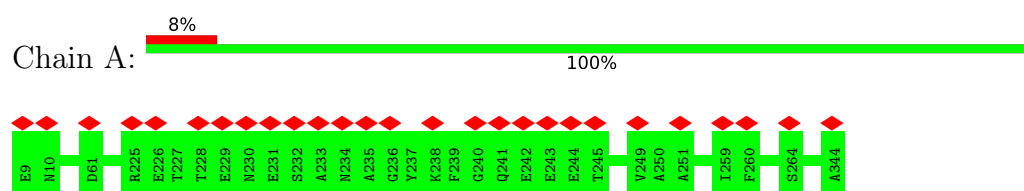


Mol	Chain	Residues	Atoms					AltConf
51	Y	1	Total	C	N	O	P	0
			69	49	2	16	2	
51	Y	1	Total	C	N	O	P	0
			69	49	2	16	2	

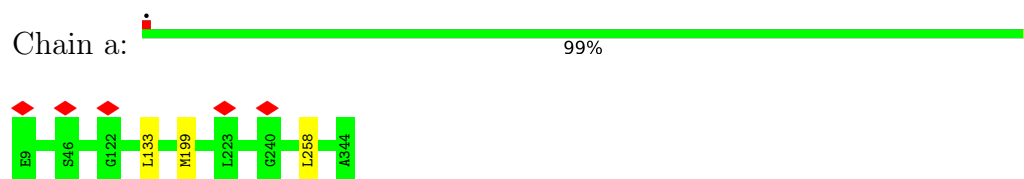
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

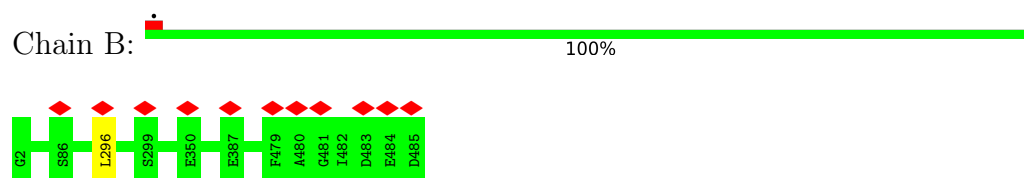
- Molecule 1: Photosystem II protein D1



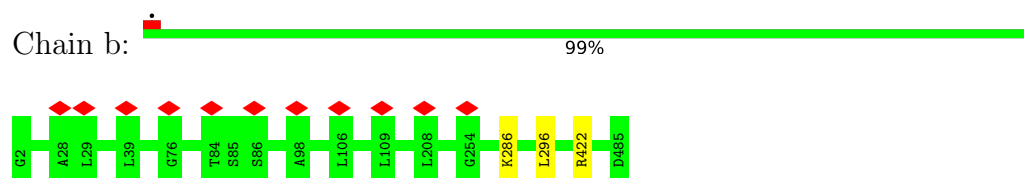
- Molecule 1: Photosystem II protein D1



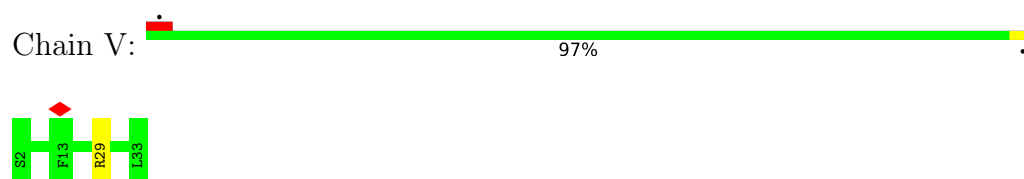
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II reaction center protein Ycf12



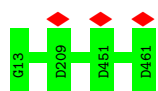
- Molecule 3: Photosystem II reaction center protein Ycf12

Chain v:  100%

There are no outlier residues recorded for this chain.

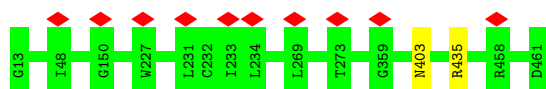
- Molecule 4: Photosystem II CP43 reaction center protein

Chain C:  100%



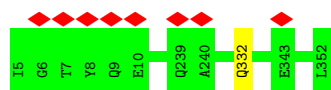
- Molecule 4: Photosystem II CP43 reaction center protein

Chain c:  100%



- Molecule 5: Photosystem II D2 protein

Chain D:  100%



- Molecule 5: Photosystem II D2 protein

Chain d:  99%



- Molecule 6: Cytochrome b559 subunit alpha

Chain E:  100%



- Molecule 6: Cytochrome b559 subunit alpha

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Cytochrome b559 subunit beta

Chain F:  100%

There are no outlier residues recorded for this chain.

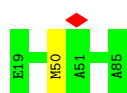
- Molecule 7: Cytochrome b559 subunit beta

Chain f:  97%



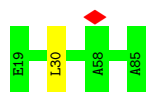
- Molecule 8: Photosystem II reaction center protein H

Chain H:  99%



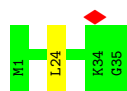
- Molecule 8: Photosystem II reaction center protein H

Chain h:  99%



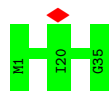
- Molecule 9: Photosystem II reaction center protein I

Chain I:  97%



- Molecule 9: Photosystem II reaction center protein I

Chain i:  100%



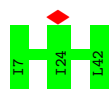
- Molecule 10: Photosystem II reaction center protein J

Chain J:  100%



- Molecule 10: Photosystem II reaction center protein J

Chain j:  100%



- Molecule 11: Photosystem II reaction center protein K

Chain K:  100%

There are no outlier residues recorded for this chain.

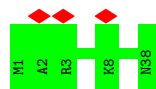
- Molecule 11: Photosystem II reaction center protein K

Chain k:  100%

There are no outlier residues recorded for this chain.

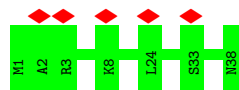
- Molecule 12: Photosystem II reaction center protein L

Chain L:  8% 100%



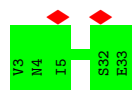
- Molecule 12: Photosystem II reaction center protein L

Chain l:  13% 100%



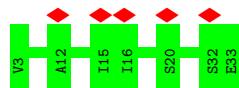
- Molecule 13: Photosystem II reaction center protein M

Chain M:  6% 100%



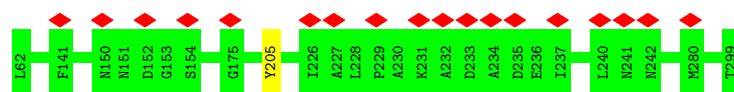
- Molecule 13: Photosystem II reaction center protein M

Chain m:  16% 100%

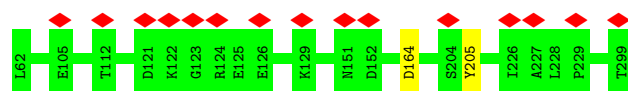


- Molecule 14: PsbO

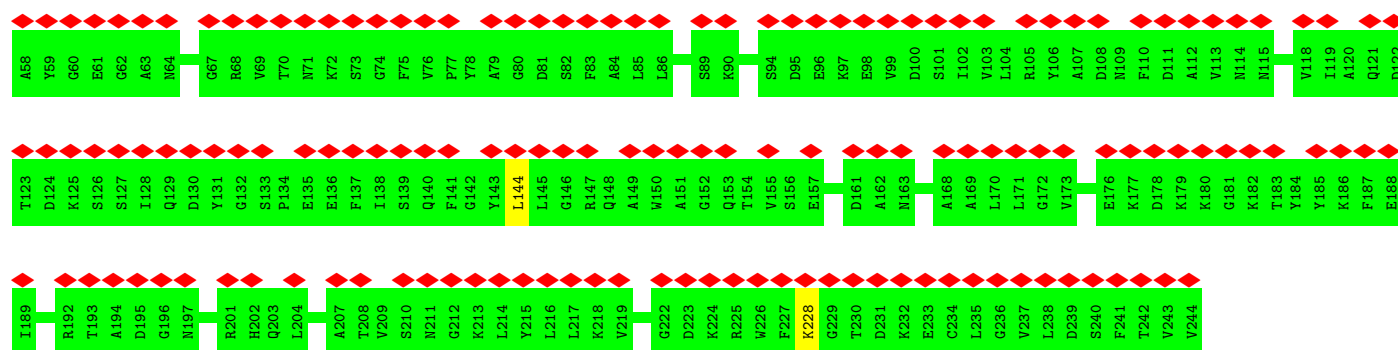
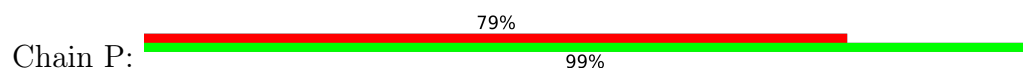
Chain O:  8% 100%



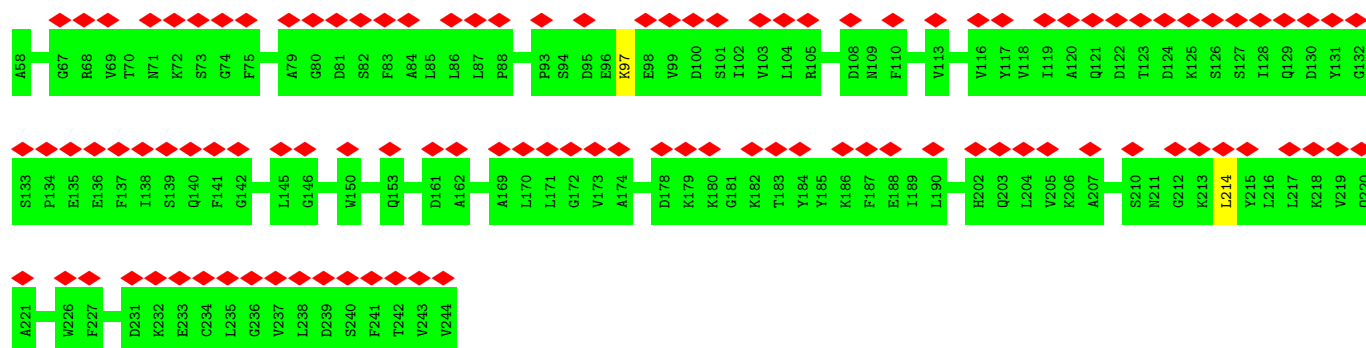
- Molecule 14: PsbO



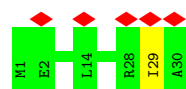
- Molecule 15: PsbP



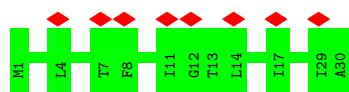
- Molecule 15: PsbP



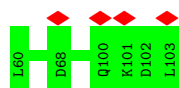
- Molecule 16: Photosystem II reaction center protein T



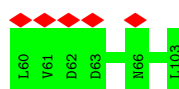
- Molecule 16: Photosystem II reaction center protein T



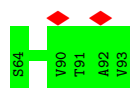
- Molecule 17: PsbW



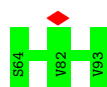
- Molecule 17: PsbW



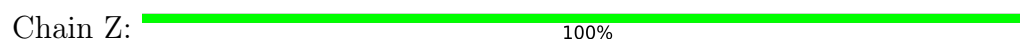
- Molecule 18: PsbX



- Molecule 18: PsbX



- Molecule 19: Photosystem II reaction center protein Z



There are no outlier residues recorded for this chain.

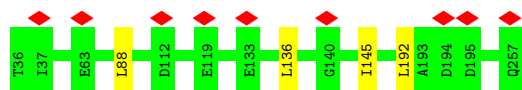
- Molecule 19: Photosystem II reaction center protein Z



There are no outlier residues recorded for this chain.

- Molecule 20: Chlorophyll a-b binding protein of LHCII type I, chloroplastic





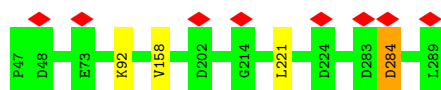
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain G: 100%



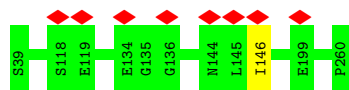
- Molecule 22: CP26

Chain S: 98%



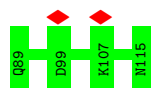
- Molecule 23: LHCII M1

Chain Y: 100%



- Molecule 24: PsbU

Chain U: 7% 100%



- Molecule 24: PsbU

Chain u: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21066	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	22.262	Depositor
Minimum map value	-13.270	Depositor
Average map value	0.035	Depositor
Map value standard deviation	1.121	Depositor
Recommended contour level	3.5	Depositor
Map size (\AA)	448.0, 448.0, 448.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.896, 0.896, 0.896	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LPX, LUT, PL9, LHG, BCT, PTY, CL, 4RF, DGA, FE2, 3PH, RRX, BCR, LMK, HEM, PHO, XAT, CHL, CLA, NEX, OEX, SQD, LMG, DGD, SPH, CSD, C7Z

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.29	0/2723	0.52	0/3715
1	a	0.33	0/2723	0.63	3/3715 (0.1%)
2	B	0.28	0/3906	0.53	1/5319 (0.0%)
2	b	0.29	0/3906	0.55	1/5319 (0.0%)
3	V	0.27	0/228	0.56	0/311
3	v	0.26	0/228	0.67	0/311
4	C	0.27	0/3602	0.51	0/4913
4	c	0.29	0/3602	0.55	0/4913
5	D	0.29	0/2860	0.53	0/3899
5	d	0.32	0/2860	0.60	2/3899 (0.1%)
6	E	0.27	0/639	0.53	0/870
6	e	0.30	0/639	0.53	0/870
7	F	0.27	0/259	0.50	0/351
7	f	0.27	0/259	0.75	1/351 (0.3%)
8	H	0.28	0/513	0.65	1/703 (0.1%)
8	h	0.29	0/513	0.69	1/703 (0.1%)
9	I	0.29	0/287	0.63	1/386 (0.3%)
9	i	0.33	0/287	0.58	0/386
10	J	0.26	0/272	0.45	0/369
10	j	0.25	0/272	0.57	0/369
11	K	0.31	0/308	0.54	0/423
11	k	0.38	0/308	0.62	0/423
12	L	0.30	0/321	0.49	0/435
12	l	0.30	0/321	0.57	0/435
13	M	0.32	0/237	0.51	0/323
13	m	0.30	0/237	0.61	0/323
14	O	0.28	0/1857	0.60	0/2508
14	o	0.27	0/1857	0.58	1/2508 (0.0%)
15	P	0.26	0/1473	0.53	1/1988 (0.1%)
15	p	0.26	0/1473	0.57	1/1988 (0.1%)
16	T	0.29	0/254	0.67	0/342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.29	0/254	0.57	0/342
17	W	0.26	0/339	0.56	0/460
17	w	0.27	0/339	0.59	0/460
18	X	0.28	0/202	0.49	0/276
18	x	0.28	0/202	0.46	0/276
19	Z	0.26	0/469	0.42	0/641
19	z	0.31	0/469	0.54	0/641
20	N	0.27	0/1751	0.55	2/2386 (0.1%)
21	G	0.27	0/1725	0.51	0/2348
22	S	0.28	0/1903	0.59	2/2590 (0.1%)
23	Y	0.26	0/1719	0.49	0/2343
24	U	0.27	0/224	0.61	0/298
24	u	0.24	0/224	0.57	0/298
All	All	0.29	0/49044	0.56	18/66727 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	c	0	1
5	d	0	1
All	All	0	2

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	296	LEU	CA-CB-CG	7.80	133.23	115.30
2	b	296	LEU	CA-CB-CG	7.76	133.15	115.30
1	a	133	LEU	CB-CG-CD2	7.16	123.17	111.00
22	S	221	LEU	CA-CB-CG	7.05	131.51	115.30
1	a	199	MET	CB-CG-SD	6.42	131.66	112.40
22	S	284	ASP	CB-CG-OD1	6.21	123.89	118.30
7	f	39	MET	CB-CG-SD	-6.06	94.23	112.40
8	H	50	MET	CB-CG-SD	-5.95	94.54	112.40
5	d	138	LEU	CA-CB-CG	5.78	128.60	115.30
1	a	258	LEU	CA-CB-CG	5.70	128.41	115.30
14	o	164	ASP	CB-CG-OD1	5.60	123.34	118.30
8	h	30	LEU	CA-CB-CG	5.47	127.89	115.30
20	N	88	LEU	CA-CB-CG	5.35	127.61	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	p	214	LEU	CA-CB-CG	5.34	127.59	115.30
9	I	24	LEU	CA-CB-CG	5.34	127.58	115.30
20	N	136	LEU	CA-CB-CG	5.18	127.20	115.30
15	P	144	LEU	CA-CB-CG	5.08	127.00	115.30
5	d	320	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	c	435	ARG	Sidechain
5	d	136	VAL	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/336 (100%)	323 (96%)	12 (4%)	0	100	100
1	a	335/336 (100%)	317 (95%)	18 (5%)	0	100	100
2	B	481/484 (99%)	463 (96%)	18 (4%)	0	100	100
2	b	481/484 (99%)	465 (97%)	16 (3%)	0	100	100
3	V	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	v	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	428 (96%)	19 (4%)	0	100	100
4	c	447/449 (100%)	420 (94%)	27 (6%)	0	100	100
5	D	346/348 (99%)	334 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	d	346/348 (99%)	329 (95%)	17 (5%)	0	100	100
6	E	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
6	e	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	h	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
9	I	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
9	i	33/35 (94%)	30 (91%)	3 (9%)	0	100	100
10	J	34/36 (94%)	34 (100%)	0	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
12	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
13	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	m	29/31 (94%)	29 (100%)	0	0	100	100
14	O	236/238 (99%)	217 (92%)	18 (8%)	1 (0%)	34	71
14	o	236/238 (99%)	215 (91%)	20 (8%)	1 (0%)	34	71
15	P	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
15	p	185/187 (99%)	168 (91%)	17 (9%)	0	100	100
16	T	28/30 (93%)	27 (96%)	0	1 (4%)	3	29
16	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
17	W	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
17	w	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
18	X	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
20	N	220/222 (99%)	204 (93%)	14 (6%)	2 (1%)	17	56
21	G	219/221 (99%)	207 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	S	241/243 (99%)	221 (92%)	17 (7%)	3 (1%)	13	51
23	Y	220/222 (99%)	207 (94%)	12 (6%)	1 (0%)	29	67
24	U	25/27 (93%)	25 (100%)	0	0	100	100
24	u	25/27 (93%)	25 (100%)	0	0	100	100
All	All	6054/6142 (99%)	5755 (95%)	290 (5%)	9 (0%)	54	83

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	O	205	TYR
20	N	192	LEU
14	o	205	TYR
22	S	284	ASP
23	Y	146	ILE
20	N	145	ILE
22	S	158	VAL
22	S	92	LYS
16	T	29	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/275 (100%)	276 (100%)	0	100	100
1	a	276/275 (100%)	276 (100%)	0	100	100
2	B	387/387 (100%)	387 (100%)	0	100	100
2	b	387/387 (100%)	385 (100%)	2 (0%)	88	95
3	V	25/25 (100%)	24 (96%)	1 (4%)	31	64
3	v	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	349 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	D	279/279 (100%)	278 (100%)	1 (0%)	91	96
5	d	279/279 (100%)	277 (99%)	2 (1%)	84	92
6	E	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100
14	O	197/197 (100%)	197 (100%)	0	100	100
14	o	197/197 (100%)	197 (100%)	0	100	100
15	P	151/151 (100%)	150 (99%)	1 (1%)	84	92
15	p	151/151 (100%)	150 (99%)	1 (1%)	84	92
16	T	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	G	168/168 (100%)	167 (99%)	1 (1%)	86	94
22	S	190/190 (100%)	190 (100%)	0	100	100
23	Y	167/167 (100%)	167 (100%)	0	100	100
24	U	26/26 (100%)	26 (100%)	0	100	100
24	u	26/26 (100%)	26 (100%)	0	100	100
All	All	4942/4940 (100%)	4932 (100%)	10 (0%)	93	98

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	V	29	ARG
5	D	332	GLN
15	P	228	LYS
21	G	73	GLN
2	b	286	LYS
2	b	422	ARG
4	c	403	ASN
5	d	83	ASN
5	d	180	ARG
15	p	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	282	GLN
5	D	332	GLN
8	H	69	ASN
14	O	274	GLN
23	Y	247	ASN
1	a	181	ASN
1	a	303	ASN
2	b	282	GLN
2	b	290	GLN
2	b	317	ASN
15	p	202	HIS
15	p	220	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSD	B	218	2	3,7,8	0.85	0	1,8,10	0.20	0
2	CSD	b	218	2	3,7,8	0.93	0	1,8,10	0.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSD	B	218	2	-	1/2/6/8	-
2	CSD	b	218	2	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	218	CSD	N-CA-CB-SG
2	b	218	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 250 ligands modelled in this entry, 6 are monoatomic - leaving 244 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	LMK	c	527	-	38,39,53	1.49	2 (5%)	41,46,60	1.26	2 (4%)
28	CLA	B	615	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	17 (22%)
32	LMG	a	413	-	48,48,55	1.00	4 (8%)	56,56,63	1.14	3 (5%)
50	LPX	S	625	-	29,29,29	1.00	2 (6%)	31,33,33	0.97	1 (3%)
32	LMG	h	102	-	48,48,55	1.01	6 (12%)	56,56,63	1.17	3 (5%)
28	CLA	S	609	-	60,68,73	1.42	9 (15%)	70,107,113	2.03	16 (22%)
28	CLA	B	616	-	65,73,73	1.37	9 (13%)	76,113,113	1.90	15 (19%)
28	CLA	A	406	-	65,73,73	1.33	6 (9%)	76,113,113	2.04	17 (22%)
28	CLA	G	602	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	18 (23%)
32	LMG	c	521	-	51,51,55	1.07	4 (7%)	59,59,63	1.01	2 (3%)
28	CLA	b	612	-	65,73,73	1.33	6 (9%)	76,113,113	2.01	16 (21%)
28	CLA	N	613	-	65,73,73	1.37	10 (15%)	76,113,113	1.99	17 (22%)
30	BCR	B	618	-	41,41,41	1.88	5 (12%)	56,56,56	4.50	16 (28%)
45	4RF	K	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.86	3 (5%)
46	CHL	N	601	-	66,74,74	0.81	3 (4%)	73,114,114	1.23	12 (16%)
28	CLA	c	512	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	18 (23%)
28	CLA	N	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	16 (21%)
28	CLA	b	605	-	65,73,73	1.38	9 (13%)	76,113,113	1.99	16 (21%)
30	BCR	c	515	-	41,41,41	1.86	4 (9%)	56,56,56	4.26	14 (25%)
38	LHG	C	525	-	46,46,48	0.40	0	49,52,54	1.02	2 (4%)
28	CLA	G	604	-	49,57,73	1.57	10 (20%)	55,93,113	2.27	19 (34%)
46	CHL	G	605	-	48,56,74	0.95	2 (4%)	51,92,114	1.41	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMG	d	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.03	2 (3%)
28	CLA	N	614	-	49,57,73	1.56	10 (20%)	55,93,113	2.31	16 (29%)
35	DGD	c	520	-	60,60,67	1.09	6 (10%)	74,74,81	0.90	2 (2%)
28	CLA	B	606	-	65,73,73	1.33	7 (10%)	76,113,113	2.10	18 (23%)
28	CLA	b	611	-	65,73,73	1.35	8 (12%)	76,113,113	2.01	17 (22%)
38	LHG	l	101	-	48,48,48	0.38	0	51,54,54	4.45	4 (7%)
49	NEX	G	623	-	38,46,46	3.25	10 (26%)	50,70,70	1.87	9 (18%)
29	PHO	a	409	-	51,69,69	0.99	3 (5%)	47,99,99	1.25	5 (10%)
46	CHL	G	601	21	66,74,74	0.82	3 (4%)	73,114,114	1.23	11 (15%)
40	BCT	D	401	-	2,3,3	1.27	0	2,3,3	4.06	2 (100%)
31	SQD	C	526	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
32	LMG	H	102	-	48,48,55	1.00	5 (10%)	56,56,63	1.11	2 (3%)
37	DGA	J	101	-	28,28,43	1.31	3 (10%)	30,30,45	1.24	2 (6%)
28	CLA	C	503	-	65,73,73	1.36	9 (13%)	76,113,113	1.99	18 (23%)
35	DGD	c	519	-	63,63,67	1.13	6 (9%)	77,77,81	0.94	2 (2%)
37	DGA	j	101	-	28,28,43	1.30	3 (10%)	30,30,45	1.20	2 (6%)
28	CLA	A	405	-	65,73,73	1.33	7 (10%)	76,113,113	1.97	17 (22%)
30	BCR	C	514	-	41,41,41	1.85	4 (9%)	56,56,56	4.41	15 (26%)
30	BCR	b	618	-	41,41,41	1.88	4 (9%)	56,56,56	4.61	20 (35%)
28	CLA	a	406	-	65,73,73	1.34	7 (10%)	76,113,113	1.93	18 (23%)
29	PHO	A	408	-	51,69,69	1.01	4 (7%)	47,99,99	1.13	6 (12%)
28	CLA	S	612	-	45,53,73	1.60	7 (15%)	52,89,113	2.17	16 (30%)
32	LMG	B	622	-	44,44,55	0.88	3 (6%)	52,52,63	1.09	2 (3%)
28	CLA	b	614	-	65,73,73	1.35	7 (10%)	76,113,113	1.98	18 (23%)
42	HEM	F	101	6,7	41,50,50	1.48	5 (12%)	45,82,82	1.38	6 (13%)
29	PHO	A	409	-	51,69,69	1.01	4 (7%)	47,99,99	1.15	5 (10%)
38	LHG	D	409	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
34	C7Z	b	620	-	43,43,43	5.37	26 (60%)	58,60,60	2.26	19 (32%)
47	LUT	N	621	-	42,43,43	2.37	1 (2%)	51,60,60	2.04	11 (21%)
43	RRX	H	101	-	42,42,42	4.83	24 (57%)	57,58,58	2.76	22 (38%)
28	CLA	B	611	-	65,73,73	1.37	8 (12%)	76,113,113	1.97	16 (21%)
38	LHG	S	624	28	44,44,48	0.41	0	47,50,54	1.12	3 (6%)
28	CLA	C	506	-	65,73,73	1.36	7 (10%)	76,113,113	1.95	16 (21%)
28	CLA	Y	610	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	20 (26%)
31	SQD	b	621	-	41,42,54	0.89	0	50,53,65	0.93	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	b	609	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	18 (23%)
28	CLA	B	603	-	65,73,73	1.36	9 (13%)	76,113,113	2.01	18 (23%)
25	OEX	A	401	1,4	0,15,15	-	-	-	-	-
28	CLA	c	508	-	65,73,73	1.34	6 (9%)	76,113,113	2.01	18 (23%)
28	CLA	b	604	-	65,73,73	1.35	8 (12%)	76,113,113	1.93	17 (22%)
28	CLA	c	509	-	65,73,73	1.35	6 (9%)	76,113,113	1.95	16 (21%)
28	CLA	B	612	-	65,73,73	1.34	7 (10%)	76,113,113	1.97	18 (23%)
28	CLA	b	615	-	65,73,73	1.35	7 (10%)	76,113,113	1.98	17 (22%)
48	XAT	Y	622	-	39,47,47	0.68	1 (2%)	54,74,74	3.70	19 (35%)
46	CHL	Y	605	23	46,54,74	0.97	2 (4%)	49,90,114	1.34	8 (16%)
46	CHL	S	607	-	43,51,74	1.02	3 (6%)	45,86,114	1.43	8 (17%)
47	LUT	Y	621	-	42,43,43	2.35	1 (2%)	51,60,60	2.02	14 (27%)
47	LUT	G	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.96	13 (25%)
36	3PH	S	626	-	47,47,47	0.86	4 (8%)	51,52,52	4.42	4 (7%)
46	CHL	Y	606	-	66,74,74	0.84	3 (4%)	73,114,114	1.19	10 (13%)
28	CLA	Y	608	-	50,58,73	1.55	10 (20%)	58,95,113	2.19	16 (27%)
35	DGD	c	518	-	56,56,67	0.98	3 (5%)	70,70,81	0.99	2 (2%)
28	CLA	B	610	-	65,73,73	1.37	7 (10%)	76,113,113	1.84	14 (18%)
28	CLA	N	604	-	65,73,73	1.35	9 (13%)	76,113,113	2.05	19 (25%)
46	CHL	N	608	-	50,58,74	0.92	2 (4%)	52,94,114	1.40	10 (19%)
28	CLA	Y	602	-	65,73,73	1.34	8 (12%)	76,113,113	1.97	19 (25%)
32	LMG	A	413	-	48,48,55	1.01	5 (10%)	56,56,63	1.17	4 (7%)
28	CLA	B	602	-	65,73,73	1.36	9 (13%)	76,113,113	1.97	17 (22%)
31	SQD	m	101	-	41,42,54	0.88	0	50,53,65	0.97	2 (4%)
39	LMK	C	527	-	38,39,53	1.51	2 (5%)	41,46,60	1.47	2 (4%)
46	CHL	N	605	20	66,74,74	0.83	2 (3%)	73,114,114	1.19	8 (10%)
30	BCR	d	404	-	41,41,41	1.87	4 (9%)	56,56,56	4.39	17 (30%)
36	3PH	B	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.12	2 (3%)
46	CHL	G	606	-	50,58,74	0.99	3 (6%)	52,94,114	1.38	8 (15%)
28	CLA	a	410	-	60,68,73	1.40	7 (11%)	70,107,113	2.05	17 (24%)
30	BCR	B	619	-	41,41,41	1.84	4 (9%)	56,56,56	4.31	18 (32%)
31	SQD	B	626	-	53,54,54	0.80	0	62,65,65	0.91	2 (3%)
42	HEM	f	101	6,7	41,50,50	1.47	5 (12%)	45,82,82	1.35	5 (11%)
46	CHL	S	606	-	44,52,74	1.06	3 (6%)	46,87,114	1.42	8 (17%)
51	PTY	Y	627	-	18,18,49	1.29	3 (16%)	21,23,54	1.41	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	LUT	Y	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.96	12 (23%)
28	CLA	S	602	-	60,68,73	1.39	8 (13%)	70,107,113	2.14	20 (28%)
32	LMG	D	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.05	2 (3%)
35	DGD	B	623	-	44,44,67	0.86	1 (2%)	58,58,81	1.14	3 (5%)
28	CLA	C	505	-	65,73,73	1.38	9 (13%)	76,113,113	1.93	17 (22%)
46	CHL	Y	601	23	66,74,74	0.80	2 (3%)	73,114,114	1.18	8 (10%)
32	LMG	w	201	-	39,39,55	0.86	2 (5%)	47,47,63	1.05	2 (4%)
28	CLA	N	602	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	17 (22%)
38	LHG	d	410	-	38,38,48	0.42	0	41,44,54	1.13	3 (7%)
28	CLA	C	507	-	65,73,73	1.37	9 (13%)	76,113,113	2.02	19 (25%)
28	CLA	C	512	-	65,73,73	1.34	7 (10%)	76,113,113	2.01	18 (23%)
38	LHG	N	624	-	48,48,48	0.38	0	51,54,54	1.07	3 (5%)
28	CLA	d	402	-	65,73,73	1.37	8 (12%)	76,113,113	1.92	19 (25%)
28	CLA	C	502	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	16 (21%)
32	LMG	C	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.09	4 (6%)
51	PTY	Y	626	-	49,49,49	0.88	4 (8%)	52,54,54	1.06	2 (3%)
28	CLA	G	613	-	65,73,73	1.37	9 (13%)	76,113,113	1.99	16 (21%)
28	CLA	b	608	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	18 (23%)
28	CLA	C	513	-	65,73,73	1.38	8 (12%)	76,113,113	1.98	15 (19%)
28	CLA	c	503	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	18 (23%)
28	CLA	b	616	-	65,73,73	1.36	8 (12%)	76,113,113	1.96	17 (22%)
28	CLA	B	607	-	65,73,73	1.35	9 (13%)	76,113,113	2.00	19 (25%)
38	LHG	L	101	-	48,48,48	0.38	0	51,54,54	4.45	5 (9%)
28	CLA	A	407	-	50,58,73	1.54	8 (16%)	58,95,113	2.25	18 (31%)
28	CLA	S	604	-	55,63,73	1.47	8 (14%)	64,101,113	2.21	18 (28%)
28	CLA	S	617	-	50,58,73	1.55	9 (18%)	58,95,113	2.26	17 (29%)
28	CLA	Y	614	-	65,73,73	1.35	8 (12%)	76,113,113	1.93	17 (22%)
45	4RF	k	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.87	3 (5%)
38	LHG	Y	624	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
35	DGD	C	519	-	63,63,67	1.13	6 (9%)	77,77,81	0.97	3 (3%)
28	CLA	G	612	-	43,51,73	1.66	8 (18%)	49,86,113	2.17	13 (26%)
28	CLA	Y	603	-	65,73,73	1.34	8 (12%)	76,113,113	2.00	18 (23%)
28	CLA	c	513	-	65,73,73	1.34	7 (10%)	76,113,113	2.09	22 (28%)
37	DGA	c	524	-	43,43,43	1.14	3 (6%)	45,45,45	1.48	3 (6%)
31	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.91	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	3PH	t	101	-	47,47,47	0.87	4 (8%)	51,52,52	1.15	2 (3%)
49	NEX	S	623	-	38,46,46	3.36	10 (26%)	50,70,70	1.72	12 (24%)
28	CLA	c	502	-	65,73,73	1.33	6 (9%)	76,113,113	2.05	18 (23%)
30	BCR	C	516	-	41,41,41	1.87	4 (9%)	56,56,56	4.42	14 (25%)
31	SQD	B	621	-	41,42,54	0.88	0	50,53,65	0.94	2 (4%)
28	CLA	G	603	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	18 (23%)
38	LHG	D	408	-	43,43,48	0.40	0	46,49,54	1.00	2 (4%)
31	SQD	A	412	-	50,51,54	0.81	0	59,62,65	0.93	3 (5%)
46	CHL	G	608	-	44,52,74	1.03	3 (6%)	46,87,114	1.39	9 (19%)
28	CLA	Y	611	-	65,73,73	1.35	9 (13%)	76,113,113	1.94	16 (21%)
28	CLA	c	511	-	65,73,73	1.35	7 (10%)	76,113,113	2.04	17 (22%)
28	CLA	B	614	-	65,73,73	1.33	6 (9%)	76,113,113	1.99	17 (22%)
28	CLA	B	608	-	65,73,73	1.37	8 (12%)	76,113,113	2.00	15 (19%)
28	CLA	G	611	-	65,73,73	1.38	9 (13%)	76,113,113	1.96	16 (21%)
28	CLA	S	613	-	55,63,73	1.48	9 (16%)	64,101,113	2.15	18 (28%)
43	RRX	h	101	-	42,42,42	4.91	24 (57%)	57,58,58	2.40	20 (35%)
48	XAT	G	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.90	13 (24%)
28	CLA	S	605	-	50,58,73	1.59	10 (20%)	58,95,113	2.25	16 (27%)
28	CLA	Y	612	-	65,73,73	1.36	9 (13%)	76,113,113	1.97	16 (21%)
33	SPH	A	414	-	19,20,20	0.65	0	18,21,21	1.06	1 (5%)
28	CLA	C	510	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	15 (19%)
31	SQD	M	101	-	41,42,54	0.89	0	50,53,65	0.96	2 (4%)
28	CLA	G	610	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	21 (27%)
28	CLA	S	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.07	17 (22%)
48	XAT	N	622	-	39,47,47	0.68	1 (2%)	54,74,74	1.96	12 (22%)
46	CHL	N	609	-	66,74,74	0.78	2 (3%)	73,114,114	1.25	13 (17%)
46	CHL	N	606	-	66,74,74	0.87	3 (4%)	73,114,114	1.17	10 (13%)
44	GOL	I	101	-	5,5,5	0.55	0	5,5,5	0.29	0
28	CLA	C	504	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	17 (22%)
28	CLA	C	508	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	18 (23%)
30	BCR	D	404	-	41,41,41	1.82	4 (9%)	56,56,56	4.24	16 (28%)
33	SPH	a	414	-	19,20,20	0.67	0	18,21,21	1.03	0
41	PL9	D	405	-	55,55,55	1.11	4 (7%)	68,69,69	1.50	13 (19%)
28	CLA	S	611	38	65,73,73	1.37	9 (13%)	76,113,113	2.01	17 (22%)
49	NEX	N	623	-	38,46,46	3.34	10 (26%)	50,70,70	1.49	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	C	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.29	15 (26%)
28	CLA	A	410	-	60,68,73	1.39	7 (11%)	70,107,113	2.12	18 (25%)
28	CLA	S	610	-	65,73,73	1.37	8 (12%)	76,113,113	1.90	19 (25%)
28	CLA	c	505	-	65,73,73	1.35	8 (12%)	76,113,113	2.13	18 (23%)
33	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.05	1 (5%)
47	LUT	S	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.94	14 (27%)
28	CLA	c	507	-	65,73,73	1.38	8 (12%)	76,113,113	1.99	17 (22%)
38	LHG	d	408	-	43,43,48	0.40	0	46,49,54	0.99	2 (4%)
32	LMG	C	521	-	51,51,55	1.06	6 (11%)	59,59,63	1.09	4 (6%)
35	DGD	C	518	-	56,56,67	1.00	4 (7%)	70,70,81	0.91	2 (2%)
30	BCR	A	411	-	41,41,41	1.85	4 (9%)	56,56,56	4.25	13 (23%)
32	LMG	c	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.06	3 (4%)
28	CLA	D	403	-	65,73,73	1.37	8 (12%)	76,113,113	2.00	16 (21%)
38	LHG	d	409	-	48,48,48	0.38	0	51,54,54	0.99	2 (3%)
28	CLA	B	617	-	65,73,73	1.35	7 (10%)	76,113,113	1.97	17 (22%)
30	BCR	b	619	-	41,41,41	1.87	4 (9%)	56,56,56	4.37	13 (23%)
31	SQD	b	626	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
41	PL9	d	405	-	55,55,55	1.16	5 (9%)	68,69,69	1.59	13 (19%)
49	NEX	Y	623	-	38,46,46	3.29	9 (23%)	50,70,70	1.80	14 (28%)
46	CHL	Y	607	-	66,74,74	0.75	2 (3%)	73,114,114	1.20	9 (12%)
38	LHG	D	410	-	38,38,48	0.42	0	41,44,54	1.18	3 (7%)
28	CLA	b	602	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	15 (19%)
28	CLA	B	609	-	65,73,73	1.33	7 (10%)	76,113,113	2.05	19 (25%)
30	BCR	a	411	-	41,41,41	1.86	4 (9%)	56,56,56	4.31	16 (28%)
28	CLA	b	607	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	17 (22%)
45	4RF	I	102	-	56,56,56	1.05	3 (5%)	59,59,59	0.88	3 (5%)
37	DGA	B	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.49	3 (6%)
28	CLA	C	509	-	65,73,73	1.34	7 (10%)	76,113,113	1.97	16 (21%)
25	OEX	a	401	1,4	0,15,15	-	-	-	-	-
28	CLA	b	610	-	65,73,73	1.34	6 (9%)	76,113,113	1.99	18 (23%)
30	BCR	c	514	-	41,41,41	1.83	4 (9%)	56,56,56	4.45	15 (26%)
47	LUT	S	621	-	42,43,43	2.34	1 (2%)	51,60,60	1.99	15 (29%)
37	DGA	b	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.52	3 (6%)
30	BCR	c	516	-	41,41,41	1.87	4 (9%)	56,56,56	4.51	16 (28%)
32	LMG	b	622	-	44,44,55	0.87	2 (4%)	52,52,63	1.11	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	G	614	-	49,57,73	1.54	9 (18%)	55,93,113	2.33	17 (30%)
40	BCT	d	401	26	2,3,3	1.16	0	2,3,3	4.43	2 (100%)
46	CHL	S	601	22	46,54,74	1.00	3 (6%)	49,90,114	1.39	9 (18%)
32	LMG	W	201	-	39,39,55	0.87	2 (5%)	47,47,63	1.15	2 (4%)
28	CLA	N	611	-	49,57,73	1.57	9 (18%)	55,93,113	2.24	16 (29%)
28	CLA	Y	613	-	65,73,73	1.35	7 (10%)	76,113,113	1.99	17 (22%)
28	CLA	S	614	-	55,63,73	1.47	8 (14%)	64,101,113	2.09	15 (23%)
35	DGD	b	623	-	44,44,67	0.87	1 (2%)	58,58,81	1.23	5 (8%)
28	CLA	c	506	-	65,73,73	1.36	7 (10%)	76,113,113	1.94	17 (22%)
28	CLA	B	604	-	65,73,73	1.37	9 (13%)	76,113,113	1.93	16 (21%)
47	LUT	G	621	-	42,43,43	2.35	1 (2%)	51,60,60	2.02	12 (23%)
31	SQD	c	526	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
28	CLA	N	612	-	45,53,73	1.63	9 (20%)	52,89,113	2.09	13 (25%)
28	CLA	a	407	-	49,57,73	1.55	8 (16%)	55,93,113	2.44	18 (32%)
34	C7Z	B	620	-	43,43,43	5.35	26 (60%)	58,60,60	2.27	22 (37%)
30	BCR	C	515	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	12 (21%)
36	3PH	b	624	-	47,47,47	0.87	4 (8%)	51,52,52	1.11	2 (3%)
28	CLA	Y	604	-	65,73,73	1.35	8 (12%)	76,113,113	1.96	18 (23%)
28	CLA	a	405	-	65,73,73	1.30	7 (10%)	76,113,113	2.03	20 (26%)
28	CLA	d	403	-	65,73,73	1.34	8 (12%)	76,113,113	2.01	17 (22%)
29	PHO	a	408	-	51,69,69	1.01	4 (7%)	47,99,99	1.04	4 (8%)
28	CLA	c	501	-	65,73,73	1.36	9 (13%)	76,113,113	1.99	17 (22%)
45	4RF	i	101	-	56,56,56	1.04	3 (5%)	59,59,59	0.89	3 (5%)
36	3PH	T	101	-	47,47,47	0.86	4 (8%)	51,52,52	1.11	2 (3%)
28	CLA	B	613	-	65,73,73	1.35	9 (13%)	76,113,113	1.93	14 (18%)
46	CHL	S	608	-	61,69,74	0.86	3 (4%)	67,108,114	1.24	10 (14%)
28	CLA	B	605	-	65,73,73	1.36	7 (10%)	76,113,113	2.13	19 (25%)
28	CLA	C	501	-	65,73,73	1.37	9 (13%)	76,113,113	2.00	18 (23%)
28	CLA	c	510	-	65,73,73	1.32	8 (12%)	76,113,113	2.02	16 (21%)
47	LUT	N	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.92	12 (23%)
28	CLA	b	613	-	65,73,73	1.36	8 (12%)	76,113,113	1.87	16 (21%)
28	CLA	c	504	-	65,73,73	1.35	7 (10%)	76,113,113	2.02	14 (18%)
46	CHL	G	607	-	66,74,74	0.78	2 (3%)	73,114,114	1.22	11 (15%)
38	LHG	G	624	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
28	CLA	b	603	-	65,73,73	1.36	9 (13%)	76,113,113	2.01	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	CHL	N	607	-	66,74,74	0.78	2 (3%)	73,114,114	1.23	10 (13%)
30	BCR	c	517	-	41,41,41	1.88	4 (9%)	56,56,56	4.48	15 (26%)
35	DGD	C	520	-	60,60,67	1.07	6 (10%)	74,74,81	0.92	2 (2%)
46	CHL	Y	609	-	66,74,74	0.84	3 (4%)	73,114,114	1.25	11 (15%)
28	CLA	N	610	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	18 (23%)
28	CLA	C	511	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	18 (23%)
28	CLA	D	402	-	65,73,73	1.37	8 (12%)	76,113,113	1.92	17 (22%)
37	DGA	C	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.52	3 (6%)
28	CLA	b	606	-	65,73,73	1.34	7 (10%)	76,113,113	2.07	17 (22%)
46	CHL	G	609	-	66,74,74	0.86	3 (4%)	73,114,114	1.22	10 (13%)
28	CLA	b	617	-	65,73,73	1.34	6 (9%)	76,113,113	1.95	17 (22%)
38	LHG	c	525	-	46,46,48	0.40	0	49,52,54	1.02	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LMK	c	527	-	2/2/6/6	12/46/46/60	-
28	CLA	B	615	-	1/1/15/20	11/37/115/115	-
32	LMG	a	413	-	-	13/43/63/70	0/1/1/1
50	LPX	S	625	-	-	12/31/31/31	-
32	LMG	h	102	-	-	11/43/63/70	0/1/1/1
28	CLA	S	609	-	1/1/14/20	10/31/109/115	-
28	CLA	B	616	-	1/1/15/20	15/37/115/115	-
28	CLA	A	406	-	1/1/15/20	19/37/115/115	-
28	CLA	G	602	-	1/1/15/20	19/37/115/115	-
32	LMG	c	521	-	-	13/46/66/70	0/1/1/1
28	CLA	b	612	-	1/1/15/20	15/37/115/115	-
28	CLA	N	613	-	1/1/15/20	17/37/115/115	-
30	BCR	B	618	-	-	7/29/63/63	0/2/2/2
46	CHL	N	601	-	4/4/20/26	8/39/137/137	-
45	4RF	K	101	-	-	32/59/59/59	-
28	CLA	c	512	-	1/1/15/20	21/37/115/115	-
28	CLA	N	603	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	b	605	-	1/1/15/20	17/37/115/115	-
30	BCR	c	515	-	-	15/29/63/63	0/2/2/2
38	LHG	C	525	-	-	32/51/51/53	-
28	CLA	G	604	-	1/1/11/20	10/18/96/115	-
46	CHL	G	605	-	4/4/16/26	6/18/116/137	-
32	LMG	d	411	-	-	8/41/61/70	0/1/1/1
28	CLA	N	614	-	1/1/11/20	7/18/96/115	-
35	DGD	c	520	-	-	7/48/88/95	0/2/2/2
28	CLA	B	606	-	1/1/15/20	15/37/115/115	-
28	CLA	b	611	-	1/1/15/20	11/37/115/115	-
38	LHG	l	101	-	-	38/53/53/53	-
49	NEX	G	623	-	-	6/27/83/83	0/3/3/3
46	CHL	G	601	21	4/4/20/26	11/39/137/137	-
29	PHO	a	409	-	-	8/37/103/103	0/5/6/6
31	SQD	C	526	-	-	17/49/69/69	0/1/1/1
32	LMG	H	102	-	-	9/43/63/70	0/1/1/1
37	DGA	J	101	-	-	10/30/30/45	-
28	CLA	C	503	-	1/1/15/20	17/37/115/115	-
35	DGD	c	519	-	-	19/51/91/95	0/2/2/2
37	DGA	j	101	-	-	14/30/30/45	-
28	CLA	A	405	-	1/1/15/20	13/37/115/115	-
30	BCR	C	514	-	-	13/29/63/63	0/2/2/2
30	BCR	b	618	-	-	7/29/63/63	0/2/2/2
28	CLA	a	406	-	1/1/15/20	15/37/115/115	-
29	PHO	A	408	-	-	13/37/103/103	0/5/6/6
28	CLA	S	612	-	1/1/11/20	5/13/91/115	-
32	LMG	B	622	-	-	12/39/59/70	0/1/1/1
28	CLA	b	614	-	1/1/15/20	12/37/115/115	-
42	HEM	F	101	6,7	-	0/12/54/54	-
29	PHO	A	409	-	-	4/37/103/103	0/5/6/6
38	LHG	D	409	-	-	28/53/53/53	-
34	C7Z	b	620	-	1/1/12/26	14/29/67/67	0/2/2/2
47	LUT	N	621	-	-	2/29/67/67	0/2/2/2
43	RRX	H	101	-	1/1/11/25	6/29/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	611	-	1/1/15/20	11/37/115/115	-
38	LHG	S	624	28	-	31/49/49/53	-
28	CLA	C	506	-	1/1/15/20	14/37/115/115	-
28	CLA	Y	610	-	1/1/15/20	15/37/115/115	-
31	SQD	b	621	-	-	18/37/57/69	0/1/1/1
28	CLA	b	609	-	1/1/15/20	20/37/115/115	-
28	CLA	B	603	-	1/1/15/20	15/37/115/115	-
28	CLA	c	508	-	1/1/15/20	10/37/115/115	-
28	CLA	b	604	-	1/1/15/20	19/37/115/115	-
28	CLA	c	509	-	1/1/15/20	14/37/115/115	-
28	CLA	B	612	-	1/1/15/20	17/37/115/115	-
28	CLA	b	615	-	1/1/15/20	13/37/115/115	-
48	XAT	Y	622	-	-	1/31/93/93	0/4/4/4
46	CHL	Y	605	23	3/3/16/26	4/15/113/137	-
46	CHL	S	607	-	3/3/15/26	0/12/110/137	-
47	LUT	Y	621	-	-	3/29/67/67	0/2/2/2
47	LUT	G	620	-	-	4/29/67/67	0/2/2/2
46	CHL	Y	606	-	4/4/20/26	7/39/137/137	-
36	3PH	S	626	-	-	25/49/49/49	-
28	CLA	Y	608	-	1/1/12/20	9/19/97/115	-
35	DGD	c	518	-	-	19/44/84/95	0/2/2/2
28	CLA	B	610	-	1/1/15/20	14/37/115/115	-
28	CLA	N	604	-	1/1/15/20	13/37/115/115	-
46	CHL	N	608	-	3/3/16/26	3/20/118/137	-
28	CLA	Y	602	-	1/1/15/20	17/37/115/115	-
39	LMK	C	527	-	2/2/6/6	15/46/46/60	-
28	CLA	B	602	-	1/1/15/20	22/37/115/115	-
46	CHL	N	605	20	4/4/20/26	2/39/137/137	-
31	SQD	m	101	-	-	20/37/57/69	0/1/1/1
32	LMG	A	413	-	-	14/43/63/70	0/1/1/1
30	BCR	d	404	-	-	13/29/63/63	0/2/2/2
46	CHL	G	606	-	3/3/16/26	5/20/118/137	-
46	CHL	S	606	-	3/3/15/26	1/13/111/137	-
28	CLA	a	410	-	1/1/14/20	7/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	B	619	-	-	6/29/63/63	0/2/2/2
31	SQD	B	626	-	-	22/49/69/69	0/1/1/1
36	3PH	B	624	-	-	28/49/49/49	-
42	HEM	f	101	6,7	-	1/12/54/54	-
51	PTY	Y	627	-	-	13/20/20/53	-
47	LUT	Y	620	-	-	3/29/67/67	0/2/2/2
28	CLA	S	602	-	1/1/14/20	18/31/109/115	-
32	LMG	D	411	-	-	10/41/61/70	0/1/1/1
35	DGD	B	623	-	-	14/32/72/95	0/2/2/2
28	CLA	C	505	-	1/1/15/20	18/37/115/115	-
46	CHL	Y	601	23	4/4/20/26	5/39/137/137	-
32	LMG	w	201	-	-	10/34/54/70	0/1/1/1
28	CLA	N	602	-	1/1/15/20	16/37/115/115	-
38	LHG	d	410	-	-	23/43/43/53	-
28	CLA	C	507	-	1/1/15/20	20/37/115/115	-
28	CLA	C	512	-	1/1/15/20	23/37/115/115	-
38	LHG	N	624	-	-	33/53/53/53	-
28	CLA	d	402	-	1/1/15/20	21/37/115/115	-
28	CLA	C	502	-	1/1/15/20	15/37/115/115	-
32	LMG	C	523	-	-	18/50/70/70	0/1/1/1
51	PTY	Y	626	-	-	21/53/53/53	-
28	CLA	G	613	-	1/1/15/20	15/37/115/115	-
28	CLA	b	608	-	1/1/15/20	26/37/115/115	-
28	CLA	C	513	-	1/1/15/20	18/37/115/115	-
28	CLA	c	503	-	1/1/15/20	20/37/115/115	-
28	CLA	b	616	-	1/1/15/20	10/37/115/115	-
28	CLA	B	607	-	1/1/15/20	13/37/115/115	-
38	LHG	L	101	-	-	42/53/53/53	-
28	CLA	A	407	-	1/1/12/20	7/19/97/115	-
28	CLA	S	604	-	1/1/13/20	9/25/103/115	-
28	CLA	S	617	-	1/1/12/20	5/19/97/115	-
28	CLA	Y	614	-	1/1/15/20	14/37/115/115	-
45	4RF	k	101	-	-	30/59/59/59	-
38	LHG	Y	624	-	-	31/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	C	519	-	-	14/51/91/95	0/2/2/2
28	CLA	G	612	-	1/1/10/20	4/11/89/115	-
28	CLA	Y	603	-	1/1/15/20	15/37/115/115	-
28	CLA	c	513	-	1/1/15/20	12/37/115/115	-
37	DGA	c	524	-	-	25/45/45/45	-
31	SQD	a	412	-	-	22/46/66/69	0/1/1/1
36	3PH	t	101	-	-	26/49/49/49	-
49	NEX	S	623	-	-	2/27/83/83	0/3/3/3
28	CLA	c	502	-	1/1/15/20	9/37/115/115	-
30	BCR	C	516	-	-	15/29/63/63	0/2/2/2
31	SQD	B	621	-	-	13/37/57/69	0/1/1/1
28	CLA	G	603	-	1/1/15/20	17/37/115/115	-
38	LHG	D	408	-	-	24/48/48/53	-
31	SQD	A	412	-	-	16/46/66/69	0/1/1/1
46	CHL	G	608	-	3/3/15/26	1/13/111/137	-
28	CLA	Y	611	-	1/1/15/20	16/37/115/115	-
28	CLA	c	511	-	1/1/15/20	16/37/115/115	-
28	CLA	B	614	-	1/1/15/20	11/37/115/115	-
28	CLA	B	608	-	1/1/15/20	25/37/115/115	-
28	CLA	G	611	-	1/1/15/20	14/37/115/115	-
28	CLA	S	613	-	1/1/13/20	9/25/103/115	-
43	RRX	h	101	-	1/1/11/25	7/29/65/65	0/2/2/2
48	XAT	G	622	-	2/2/12/26	0/31/93/93	0/4/4/4
28	CLA	S	605	-	1/1/12/20	10/19/97/115	-
28	CLA	Y	612	-	1/1/15/20	13/37/115/115	-
33	SPH	A	414	-	-	8/21/21/21	-
28	CLA	C	510	-	1/1/15/20	16/37/115/115	-
31	SQD	M	101	-	-	18/37/57/69	0/1/1/1
28	CLA	G	610	-	1/1/15/20	18/37/115/115	-
28	CLA	S	603	-	1/1/15/20	18/37/115/115	-
48	XAT	N	622	-	1/1/12/26	0/31/93/93	0/4/4/4
46	CHL	N	609	-	4/4/20/26	6/39/137/137	-
46	CHL	N	606	-	4/4/20/26	11/39/137/137	-
44	GOL	I	101	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	C	504	-	1/1/15/20	13/37/115/115	-
28	CLA	C	508	-	1/1/15/20	13/37/115/115	-
30	BCR	D	404	-	-	12/29/63/63	0/2/2/2
33	SPH	a	414	-	-	13/21/21/21	-
41	PL9	D	405	-	-	7/53/73/73	0/1/1/1
28	CLA	S	611	38	1/1/15/20	15/37/115/115	-
49	NEX	N	623	-	-	2/27/83/83	1/3/3/3
30	BCR	C	517	-	-	10/29/63/63	0/2/2/2
28	CLA	A	410	-	1/1/14/20	11/31/109/115	-
28	CLA	S	610	-	1/1/15/20	21/37/115/115	-
28	CLA	c	505	-	1/1/15/20	17/37/115/115	-
33	SPH	Y	625	-	-	11/21/21/21	-
47	LUT	S	620	-	-	4/29/67/67	0/2/2/2
28	CLA	c	507	-	1/1/15/20	16/37/115/115	-
38	LHG	d	408	-	-	30/48/48/53	-
32	LMG	C	521	-	-	13/46/66/70	0/1/1/1
35	DGD	C	518	-	-	15/44/84/95	0/2/2/2
30	BCR	A	411	-	-	11/29/63/63	0/2/2/2
32	LMG	c	523	-	-	14/50/70/70	0/1/1/1
28	CLA	D	403	-	1/1/15/20	14/37/115/115	-
38	LHG	d	409	-	-	28/53/53/53	-
28	CLA	B	617	-	1/1/15/20	17/37/115/115	-
30	BCR	b	619	-	-	11/29/63/63	0/2/2/2
31	SQD	b	626	-	-	21/49/69/69	0/1/1/1
41	PL9	d	405	-	-	21/53/73/73	0/1/1/1
49	NEX	Y	623	-	-	5/27/83/83	0/3/3/3
46	CHL	Y	607	-	4/4/20/26	7/39/137/137	-
38	LHG	D	410	-	-	30/43/43/53	-
28	CLA	b	602	-	1/1/15/20	26/37/115/115	-
28	CLA	B	609	-	1/1/15/20	15/37/115/115	-
30	BCR	a	411	-	-	10/29/63/63	0/2/2/2
28	CLA	b	607	-	1/1/15/20	9/37/115/115	-
45	4RF	I	102	-	-	28/59/59/59	-
37	DGA	B	625	-	-	25/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	C	509	-	1/1/15/20	18/37/115/115	-
28	CLA	b	610	-	1/1/15/20	14/37/115/115	-
30	BCR	c	514	-	-	12/29/63/63	0/2/2/2
47	LUT	S	621	-	-	1/29/67/67	0/2/2/2
37	DGA	b	625	-	-	28/45/45/45	-
30	BCR	c	516	-	-	14/29/63/63	0/2/2/2
32	LMG	b	622	-	-	11/39/59/70	0/1/1/1
28	CLA	G	614	-	1/1/11/20	10/18/96/115	-
46	CHL	S	601	22	3/3/16/26	3/15/113/137	-
32	LMG	W	201	-	-	12/34/54/70	0/1/1/1
28	CLA	N	611	-	1/1/11/20	11/18/96/115	-
28	CLA	Y	613	-	1/1/15/20	20/37/115/115	-
28	CLA	S	614	-	1/1/13/20	7/25/103/115	-
35	DGD	b	623	-	-	11/32/72/95	0/2/2/2
28	CLA	c	506	-	1/1/15/20	17/37/115/115	-
28	CLA	B	604	-	1/1/15/20	17/37/115/115	-
47	LUT	G	621	-	-	5/29/67/67	0/2/2/2
31	SQD	c	526	-	-	13/49/69/69	0/1/1/1
28	CLA	N	612	-	1/1/11/20	3/13/91/115	-
28	CLA	a	407	-	1/1/11/20	9/18/96/115	-
34	C7Z	B	620	-	1/1/12/26	11/29/67/67	0/2/2/2
30	BCR	C	515	-	-	11/29/63/63	0/2/2/2
36	3PH	b	624	-	-	21/49/49/49	-
28	CLA	Y	604	-	1/1/15/20	15/37/115/115	-
28	CLA	a	405	-	1/1/15/20	13/37/115/115	-
28	CLA	d	403	-	1/1/15/20	21/37/115/115	-
29	PHO	a	408	-	-	6/37/103/103	0/5/6/6
28	CLA	c	501	-	1/1/15/20	20/37/115/115	-
45	4RF	i	101	-	-	31/59/59/59	-
36	3PH	T	101	-	-	22/49/49/49	-
28	CLA	B	613	-	1/1/15/20	16/37/115/115	-
46	CHL	S	608	-	4/4/19/26	8/33/131/137	-
28	CLA	B	605	-	1/1/15/20	14/37/115/115	-
28	CLA	C	501	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	c	510	-	1/1/15/20	18/37/115/115	-
47	LUT	N	620	-	-	3/29/67/67	0/2/2/2
28	CLA	b	613	-	1/1/15/20	17/37/115/115	-
28	CLA	c	504	-	1/1/15/20	21/37/115/115	-
46	CHL	G	607	-	4/4/20/26	10/39/137/137	-
38	LHG	G	624	-	-	29/53/53/53	-
28	CLA	b	603	-	1/1/15/20	16/37/115/115	-
46	CHL	N	607	-	4/4/20/26	11/39/137/137	-
30	BCR	c	517	-	-	8/29/63/63	0/2/2/2
35	DGD	C	520	-	-	8/48/88/95	0/2/2/2
46	CHL	Y	609	-	4/4/20/26	11/39/137/137	-
28	CLA	N	610	-	1/1/15/20	22/37/115/115	-
28	CLA	C	511	-	1/1/15/20	11/37/115/115	-
28	CLA	D	402	-	1/1/15/20	20/37/115/115	-
37	DGA	C	524	-	-	22/45/45/45	-
28	CLA	b	606	-	1/1/15/20	14/37/115/115	-
46	CHL	G	609	-	4/4/20/26	8/39/137/137	-
28	CLA	b	617	-	1/1/15/20	13/37/115/115	-
38	LHG	c	525	-	-	31/51/51/53	-

All (1292) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	620	C7Z	C25-C26	15.90	1.62	1.34
34	B	620	C7Z	C25-C26	15.72	1.61	1.34
43	h	101	RRX	C26-C25	15.50	1.61	1.34
43	H	101	RRX	C26-C25	15.18	1.60	1.34
34	b	620	C7Z	C5-C6	15.02	1.60	1.34
43	h	101	RRX	C5-C6	15.01	1.60	1.34
34	B	620	C7Z	C5-C6	14.94	1.60	1.34
43	H	101	RRX	C5-C6	14.75	1.60	1.34
47	N	620	LUT	C24-C25	14.69	1.51	1.33
47	Y	620	LUT	C24-C25	14.53	1.51	1.33
47	N	621	LUT	C24-C25	14.52	1.51	1.33
47	G	620	LUT	C24-C25	14.48	1.51	1.33
47	Y	621	LUT	C24-C25	14.45	1.51	1.33
47	G	621	LUT	C24-C25	14.44	1.51	1.33
47	S	620	LUT	C24-C25	14.42	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S	621	LUT	C24-C25	14.38	1.51	1.33
34	B	620	C7Z	C24-C23	11.77	1.72	1.52
34	b	620	C7Z	C24-C23	11.76	1.72	1.52
43	H	101	RRX	C29-C28	-10.40	1.37	1.52
43	h	101	RRX	C29-C28	-10.39	1.37	1.52
34	B	620	C7Z	C22-C23	-10.25	1.37	1.52
34	b	620	C7Z	C2-C3	-10.24	1.37	1.52
34	b	620	C7Z	C22-C23	-10.23	1.37	1.52
34	B	620	C7Z	C2-C3	-10.21	1.37	1.52
34	B	620	C7Z	C4-C3	8.64	1.67	1.52
34	b	620	C7Z	C4-C3	8.61	1.67	1.52
43	h	101	RRX	C27-C28	7.78	1.65	1.52
49	S	623	NEX	C14-C13	-7.74	1.25	1.35
49	S	623	NEX	C30-C29	-7.63	1.25	1.35
30	c	515	BCR	C10-C9	7.59	1.45	1.35
49	N	623	NEX	C14-C13	-7.57	1.25	1.35
49	G	623	NEX	C34-C33	-7.56	1.25	1.35
30	C	516	BCR	C10-C9	7.56	1.45	1.35
49	S	623	NEX	C34-C33	-7.55	1.25	1.35
49	N	623	NEX	C30-C29	-7.52	1.25	1.35
30	c	517	BCR	C10-C9	7.48	1.45	1.35
49	N	623	NEX	C34-C33	-7.47	1.25	1.35
43	H	101	RRX	C27-C28	7.45	1.65	1.52
30	d	404	BCR	C10-C9	7.44	1.45	1.35
49	G	623	NEX	C30-C29	-7.43	1.25	1.35
30	c	516	BCR	C10-C9	7.42	1.45	1.35
49	Y	623	NEX	C34-C33	-7.36	1.26	1.35
49	S	623	NEX	C10-C9	-7.30	1.26	1.35
49	G	623	NEX	C14-C13	-7.29	1.26	1.35
49	Y	623	NEX	C14-C13	-7.29	1.26	1.35
49	Y	623	NEX	C30-C29	-7.26	1.26	1.35
49	Y	623	NEX	C10-C9	-7.25	1.26	1.35
49	N	623	NEX	C10-C9	-7.23	1.26	1.35
30	b	618	BCR	C10-C9	7.17	1.45	1.35
30	c	514	BCR	C10-C9	7.16	1.45	1.35
30	A	411	BCR	C10-C9	7.15	1.45	1.35
39	C	527	LMK	O3-C4	7.14	1.43	1.22
30	C	517	BCR	C10-C9	7.13	1.45	1.35
30	b	619	BCR	C10-C9	7.13	1.45	1.35
39	c	527	LMK	O3-C4	7.09	1.43	1.22
30	a	411	BCR	C10-C9	7.09	1.45	1.35
30	C	514	BCR	C10-C9	7.04	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	618	BCR	C10-C9	6.97	1.45	1.35
30	D	404	BCR	C10-C9	6.93	1.45	1.35
30	B	619	BCR	C10-C9	6.85	1.44	1.35
30	C	515	BCR	C10-C9	6.83	1.44	1.35
49	S	623	NEX	C35-C15	-6.78	1.18	1.36
49	N	623	NEX	C35-C15	-6.76	1.18	1.36
49	Y	623	NEX	C35-C15	-6.67	1.18	1.36
49	G	623	NEX	C35-C15	-6.66	1.18	1.36
43	h	101	RRX	C2-C3	-6.56	1.36	1.52
28	S	605	CLA	MG-NA	6.49	2.21	2.06
28	S	603	CLA	MG-NA	6.48	2.21	2.06
28	c	511	CLA	MG-NA	6.47	2.21	2.06
28	c	503	CLA	MG-NA	6.47	2.21	2.06
28	G	611	CLA	MG-NA	6.45	2.21	2.06
28	N	613	CLA	MG-NA	6.44	2.21	2.06
28	Y	608	CLA	MG-NA	6.44	2.21	2.06
28	N	612	CLA	MG-NA	6.44	2.21	2.06
28	G	613	CLA	MG-NA	6.43	2.21	2.06
28	C	501	CLA	MG-NA	6.43	2.21	2.06
28	C	503	CLA	MG-NA	6.43	2.21	2.06
28	B	602	CLA	MG-NA	6.42	2.21	2.06
28	B	616	CLA	MG-NA	6.42	2.21	2.06
28	B	611	CLA	MG-NA	6.41	2.21	2.06
43	H	101	RRX	C2-C3	-6.41	1.36	1.52
28	b	616	CLA	MG-NA	6.41	2.21	2.06
28	C	511	CLA	MG-NA	6.41	2.21	2.06
28	a	407	CLA	MG-NA	6.40	2.21	2.06
28	a	406	CLA	MG-NA	6.40	2.21	2.06
28	B	608	CLA	MG-NA	6.39	2.21	2.06
28	C	512	CLA	MG-NA	6.39	2.21	2.06
28	Y	612	CLA	MG-NA	6.39	2.21	2.06
28	C	507	CLA	MG-NA	6.38	2.21	2.06
28	N	611	CLA	MG-NA	6.38	2.21	2.06
28	S	617	CLA	MG-NA	6.38	2.21	2.06
28	a	410	CLA	MG-NA	6.38	2.21	2.06
49	S	623	NEX	C31-C32	-6.38	1.18	1.34
28	B	605	CLA	MG-NA	6.37	2.21	2.06
28	N	614	CLA	MG-NA	6.37	2.21	2.06
28	b	602	CLA	MG-NA	6.37	2.21	2.06
28	S	611	CLA	MG-NA	6.37	2.21	2.06
28	b	614	CLA	MG-NA	6.37	2.21	2.06
28	B	603	CLA	MG-NA	6.36	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	407	CLA	MG-NA	6.36	2.21	2.06
28	b	605	CLA	MG-NA	6.36	2.21	2.06
28	S	613	CLA	MG-NA	6.36	2.21	2.06
28	G	612	CLA	MG-NA	6.35	2.21	2.06
28	B	615	CLA	MG-NA	6.35	2.21	2.06
28	G	604	CLA	MG-NA	6.34	2.21	2.06
28	c	512	CLA	MG-NA	6.34	2.21	2.06
28	c	501	CLA	MG-NA	6.34	2.21	2.06
28	Y	611	CLA	MG-NA	6.34	2.21	2.06
28	Y	613	CLA	MG-NA	6.34	2.21	2.06
28	c	502	CLA	MG-NA	6.34	2.21	2.06
28	B	604	CLA	MG-NA	6.33	2.21	2.06
28	C	513	CLA	MG-NA	6.32	2.21	2.06
28	N	603	CLA	MG-NA	6.32	2.21	2.06
28	S	609	CLA	MG-NA	6.32	2.21	2.06
28	b	608	CLA	MG-NA	6.31	2.21	2.06
28	b	611	CLA	MG-NA	6.31	2.21	2.06
28	N	604	CLA	MG-NA	6.31	2.21	2.06
28	S	612	CLA	MG-NA	6.29	2.21	2.06
49	S	623	NEX	C11-C12	-6.29	1.18	1.34
28	c	506	CLA	MG-NA	6.29	2.21	2.06
28	c	513	CLA	MG-NA	6.29	2.21	2.06
28	Y	602	CLA	MG-NA	6.29	2.21	2.06
49	N	623	NEX	C31-C32	-6.29	1.18	1.34
49	G	623	NEX	C31-C32	-6.29	1.18	1.34
28	Y	604	CLA	MG-NA	6.28	2.21	2.06
28	d	402	CLA	MG-NA	6.28	2.21	2.06
28	b	615	CLA	MG-NA	6.28	2.21	2.06
28	D	402	CLA	MG-NA	6.28	2.21	2.06
28	S	610	CLA	MG-NA	6.27	2.21	2.06
28	b	609	CLA	MG-NA	6.27	2.21	2.06
28	c	509	CLA	MG-NA	6.27	2.21	2.06
28	c	507	CLA	MG-NA	6.27	2.21	2.06
49	N	623	NEX	C11-C12	-6.27	1.18	1.34
28	Y	603	CLA	MG-NA	6.27	2.21	2.06
28	B	617	CLA	MG-NA	6.27	2.21	2.06
28	G	602	CLA	MG-NA	6.26	2.21	2.06
28	G	614	CLA	MG-NA	6.26	2.21	2.06
28	Y	614	CLA	MG-NA	6.26	2.21	2.06
28	N	602	CLA	MG-NA	6.26	2.21	2.06
28	C	502	CLA	MG-NA	6.26	2.21	2.06
28	G	603	CLA	MG-NA	6.26	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	403	CLA	MG-NA	6.26	2.21	2.06
28	C	506	CLA	MG-NA	6.26	2.21	2.06
28	c	504	CLA	MG-NA	6.25	2.21	2.06
28	b	604	CLA	MG-NA	6.25	2.21	2.06
28	G	610	CLA	MG-NA	6.25	2.21	2.06
28	S	602	CLA	MG-NA	6.25	2.21	2.06
28	B	609	CLA	MG-NA	6.25	2.21	2.06
28	C	505	CLA	MG-NA	6.25	2.21	2.06
28	b	613	CLA	MG-NA	6.24	2.21	2.06
28	b	617	CLA	MG-NA	6.24	2.21	2.06
28	S	604	CLA	MG-NA	6.24	2.21	2.06
28	B	614	CLA	MG-NA	6.24	2.21	2.06
28	b	607	CLA	MG-NA	6.23	2.21	2.06
49	Y	623	NEX	C11-C12	-6.22	1.18	1.34
49	G	623	NEX	C10-C9	-6.22	1.27	1.35
28	B	607	CLA	MG-NA	6.22	2.21	2.06
28	Y	610	CLA	MG-NA	6.22	2.21	2.06
28	N	610	CLA	MG-NA	6.22	2.21	2.06
28	b	603	CLA	MG-NA	6.22	2.21	2.06
28	C	504	CLA	MG-NA	6.22	2.21	2.06
28	S	614	CLA	MG-NA	6.22	2.21	2.06
28	B	610	CLA	MG-NA	6.21	2.21	2.06
28	A	410	CLA	MG-NA	6.21	2.21	2.06
28	C	509	CLA	MG-NA	6.20	2.21	2.06
49	G	623	NEX	C11-C12	-6.20	1.18	1.34
49	Y	623	NEX	C31-C32	-6.20	1.18	1.34
28	B	613	CLA	MG-NA	6.20	2.21	2.06
28	C	508	CLA	MG-NA	6.18	2.21	2.06
28	c	505	CLA	MG-NA	6.17	2.20	2.06
28	d	403	CLA	MG-NA	6.17	2.20	2.06
28	A	406	CLA	MG-NA	6.16	2.20	2.06
28	b	606	CLA	MG-NA	6.15	2.20	2.06
28	B	612	CLA	MG-NA	6.14	2.20	2.06
28	A	405	CLA	MG-NA	6.14	2.20	2.06
43	H	101	RRX	C1-C6	-6.13	1.45	1.53
28	c	510	CLA	MG-NA	6.13	2.20	2.06
28	b	610	CLA	MG-NA	6.13	2.20	2.06
28	B	606	CLA	MG-NA	6.12	2.20	2.06
28	C	510	CLA	MG-NA	6.11	2.20	2.06
28	a	405	CLA	MG-NA	6.07	2.20	2.06
28	b	612	CLA	MG-NA	6.05	2.20	2.06
28	c	508	CLA	MG-NA	5.97	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	619	BCR	C24-C23	5.93	1.51	1.33
30	d	404	BCR	C24-C23	5.84	1.50	1.33
30	C	516	BCR	C24-C23	5.80	1.50	1.33
30	c	516	BCR	C24-C23	5.80	1.50	1.33
30	c	517	BCR	C24-C23	5.78	1.50	1.33
34	b	620	C7Z	C12-C13	5.78	1.58	1.45
30	b	618	BCR	C24-C23	5.77	1.50	1.33
30	B	618	BCR	C24-C23	5.76	1.50	1.33
30	c	515	BCR	C24-C23	5.73	1.50	1.33
30	D	404	BCR	C24-C23	5.72	1.50	1.33
30	a	411	BCR	C24-C23	5.70	1.50	1.33
30	A	411	BCR	C24-C23	5.70	1.50	1.33
30	B	619	BCR	C24-C23	5.67	1.50	1.33
30	c	514	BCR	C24-C23	5.65	1.50	1.33
30	C	517	BCR	C24-C23	5.64	1.50	1.33
30	C	514	BCR	C24-C23	5.62	1.50	1.33
34	B	620	C7Z	C12-C13	5.60	1.58	1.45
30	C	515	BCR	C24-C23	5.59	1.50	1.33
43	h	101	RRX	C1-C6	-5.54	1.46	1.53
34	B	620	C7Z	C1-C6	-5.47	1.46	1.53
49	Y	623	NEX	C7-C8	5.46	1.41	1.32
49	N	623	NEX	C7-C8	5.44	1.41	1.32
34	b	620	C7Z	C1-C6	-5.39	1.46	1.53
49	S	623	NEX	C28-C29	-5.32	1.34	1.45
30	C	515	BCR	C11-C12	-5.28	1.21	1.34
30	B	619	BCR	C11-C12	-5.28	1.21	1.34
30	b	618	BCR	C11-C12	-5.27	1.21	1.34
49	N	623	NEX	C28-C29	-5.23	1.34	1.45
30	C	514	BCR	C11-C12	-5.21	1.21	1.34
49	Y	623	NEX	C28-C29	-5.20	1.34	1.45
43	H	101	RRX	C2-C1	5.19	1.66	1.54
49	G	623	NEX	C28-C29	-5.18	1.34	1.45
30	A	411	BCR	C11-C12	-5.18	1.21	1.34
30	C	517	BCR	C11-C12	-5.18	1.21	1.34
30	a	411	BCR	C11-C12	-5.17	1.21	1.34
43	h	101	RRX	C8-C9	5.17	1.57	1.45
30	b	619	BCR	C11-C12	-5.16	1.21	1.34
30	c	514	BCR	C11-C12	-5.15	1.21	1.34
34	B	620	C7Z	C28-C29	5.13	1.57	1.45
30	D	404	BCR	C11-C12	-5.13	1.21	1.34
30	B	618	BCR	C11-C12	-5.12	1.21	1.34
34	b	620	C7Z	C28-C29	5.11	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	h	101	RRX	C19-C18	5.10	1.56	1.45
43	h	101	RRX	C2-C1	5.07	1.65	1.54
30	c	517	BCR	C11-C12	-5.02	1.21	1.34
30	d	404	BCR	C11-C12	-5.01	1.21	1.34
30	c	516	BCR	C11-C12	-5.00	1.21	1.34
30	C	516	BCR	C11-C12	-4.97	1.21	1.34
43	H	101	RRX	C19-C18	4.93	1.56	1.45
49	S	623	NEX	C7-C8	4.85	1.40	1.32
34	B	620	C7Z	C24-C25	-4.81	1.43	1.51
34	b	620	C7Z	C32-C33	4.81	1.56	1.45
30	c	515	BCR	C11-C12	-4.80	1.22	1.34
34	B	620	C7Z	C32-C33	4.76	1.56	1.45
34	b	620	C7Z	C24-C25	-4.69	1.43	1.51
49	G	623	NEX	C7-C8	4.68	1.39	1.32
43	H	101	RRX	C8-C9	4.66	1.55	1.45
43	H	101	RRX	C27-C26	-4.64	1.43	1.51
43	h	101	RRX	C30-C25	-4.62	1.47	1.53
43	H	101	RRX	C30-C25	-4.60	1.47	1.53
43	h	101	RRX	C27-C26	-4.45	1.44	1.51
43	h	101	RRX	C12-C13	4.44	1.55	1.45
43	h	101	RRX	C23-C22	4.42	1.55	1.45
34	B	620	C7Z	C31-C30	4.41	1.57	1.43
34	b	620	C7Z	C31-C30	4.40	1.57	1.43
30	B	619	BCR	C16-C17	-4.40	1.29	1.43
30	C	515	BCR	C16-C17	-4.39	1.29	1.43
34	b	620	C7Z	C8-C9	4.37	1.55	1.45
35	c	520	DGD	O1G-C1A	4.36	1.46	1.33
35	b	623	DGD	O1G-C1A	4.36	1.46	1.33
34	B	620	C7Z	C4-C5	-4.34	1.44	1.51
35	B	623	DGD	O1G-C1A	4.33	1.46	1.33
30	C	514	BCR	C16-C17	-4.30	1.30	1.43
30	B	618	BCR	C16-C17	-4.30	1.30	1.43
30	a	411	BCR	C16-C17	-4.30	1.30	1.43
30	A	411	BCR	C16-C17	-4.29	1.30	1.43
43	H	101	RRX	C3-C4	4.28	1.65	1.52
34	B	620	C7Z	C8-C9	4.27	1.55	1.45
35	C	518	DGD	O1G-C1A	4.27	1.45	1.33
30	D	404	BCR	C16-C17	-4.26	1.30	1.43
30	C	517	BCR	C16-C17	-4.26	1.30	1.43
35	c	519	DGD	O1G-C1A	4.25	1.45	1.33
43	H	101	RRX	C12-C13	4.25	1.55	1.45
35	C	519	DGD	O1G-C1A	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	518	DGD	O1G-C1A	4.24	1.45	1.33
34	b	620	C7Z	C4-C5	-4.24	1.44	1.51
35	C	520	DGD	O1G-C1A	4.23	1.45	1.33
28	C	505	CLA	MG-ND	-4.23	1.97	2.05
30	b	619	BCR	C16-C17	-4.23	1.30	1.43
28	C	513	CLA	MG-ND	-4.22	1.97	2.05
34	b	620	C7Z	C11-C10	4.20	1.56	1.43
30	c	517	BCR	C16-C17	-4.18	1.30	1.43
30	c	514	BCR	C16-C17	-4.16	1.30	1.43
28	D	402	CLA	MG-ND	-4.16	1.97	2.05
30	b	618	BCR	C16-C17	-4.15	1.30	1.43
43	h	101	RRX	C3-C4	4.15	1.65	1.52
30	c	515	BCR	C16-C17	-4.13	1.30	1.43
30	d	404	BCR	C16-C17	-4.13	1.30	1.43
34	B	620	C7Z	C11-C10	4.12	1.56	1.43
30	C	516	BCR	C16-C17	-4.11	1.30	1.43
30	c	516	BCR	C16-C17	-4.10	1.30	1.43
28	C	507	CLA	MG-ND	-4.09	1.97	2.05
43	H	101	RRX	C23-C22	4.08	1.54	1.45
28	c	507	CLA	MG-ND	-4.08	1.97	2.05
42	F	101	HEM	C3C-CAC	4.07	1.56	1.47
39	C	527	LMK	O2-C4	4.05	1.43	1.30
28	b	613	CLA	MG-ND	-4.05	1.97	2.05
28	C	508	CLA	MG-ND	-4.04	1.97	2.05
28	C	506	CLA	MG-ND	-4.02	1.97	2.05
28	B	613	CLA	MG-ND	-4.00	1.97	2.05
39	c	527	LMK	O2-C4	3.99	1.43	1.30
42	f	101	HEM	C3C-CAC	3.99	1.56	1.47
28	c	505	CLA	MG-ND	-3.98	1.97	2.05
41	d	405	PL9	C7-C3	-3.98	1.47	1.51
28	b	612	CLA	MG-ND	-3.97	1.97	2.05
34	B	620	C7Z	C22-C21	3.97	1.67	1.54
28	B	612	CLA	MG-ND	-3.96	1.97	2.05
28	b	604	CLA	MG-ND	-3.96	1.97	2.05
28	S	611	CLA	MG-ND	-3.95	1.98	2.05
28	b	617	CLA	MG-ND	-3.95	1.98	2.05
28	A	405	CLA	MG-ND	-3.95	1.98	2.05
28	B	617	CLA	MG-ND	-3.94	1.98	2.05
28	B	604	CLA	MG-ND	-3.94	1.98	2.05
28	d	402	CLA	MG-ND	-3.94	1.98	2.05
43	h	101	RRX	C20-C21	3.93	1.55	1.43
34	b	620	C7Z	C22-C21	3.92	1.67	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	504	CLA	MG-ND	-3.92	1.98	2.05
28	A	410	CLA	MG-ND	-3.92	1.98	2.05
28	b	611	CLA	MG-ND	-3.91	1.98	2.05
28	b	607	CLA	MG-ND	-3.91	1.98	2.05
28	c	506	CLA	MG-ND	-3.91	1.98	2.05
28	b	609	CLA	MG-ND	-3.91	1.98	2.05
28	a	410	CLA	MG-ND	-3.91	1.98	2.05
28	S	605	CLA	MG-ND	-3.90	1.98	2.05
28	a	406	CLA	MG-ND	-3.90	1.98	2.05
28	C	509	CLA	MG-ND	-3.90	1.98	2.05
43	h	101	RRX	C15-C14	3.89	1.55	1.43
28	C	512	CLA	MG-ND	-3.89	1.98	2.05
28	b	605	CLA	MG-ND	-3.89	1.98	2.05
28	c	508	CLA	MG-ND	-3.89	1.98	2.05
28	B	609	CLA	MG-ND	-3.88	1.98	2.05
28	B	611	CLA	MG-ND	-3.88	1.98	2.05
28	N	604	CLA	MG-ND	-3.87	1.98	2.05
28	B	608	CLA	MG-ND	-3.87	1.98	2.05
28	Y	608	CLA	MG-ND	-3.87	1.98	2.05
28	G	604	CLA	MG-ND	-3.87	1.98	2.05
28	S	603	CLA	MG-ND	-3.86	1.98	2.05
28	B	605	CLA	MG-ND	-3.86	1.98	2.05
28	a	407	CLA	MG-ND	-3.86	1.98	2.05
28	N	613	CLA	MG-ND	-3.85	1.98	2.05
28	B	610	CLA	MG-ND	-3.85	1.98	2.05
28	G	602	CLA	MG-ND	-3.85	1.98	2.05
28	S	614	CLA	MG-ND	-3.85	1.98	2.05
28	b	608	CLA	MG-ND	-3.85	1.98	2.05
28	B	615	CLA	MG-ND	-3.84	1.98	2.05
28	B	607	CLA	MG-ND	-3.84	1.98	2.05
28	c	502	CLA	MG-ND	-3.83	1.98	2.05
34	B	620	C7Z	C15-C14	3.83	1.55	1.43
28	c	512	CLA	MG-ND	-3.83	1.98	2.05
28	S	617	CLA	MG-ND	-3.83	1.98	2.05
28	A	406	CLA	MG-ND	-3.83	1.98	2.05
28	C	503	CLA	MG-ND	-3.83	1.98	2.05
28	b	603	CLA	MG-ND	-3.83	1.98	2.05
28	C	510	CLA	MG-ND	-3.83	1.98	2.05
28	b	615	CLA	MG-ND	-3.83	1.98	2.05
28	b	614	CLA	MG-ND	-3.82	1.98	2.05
28	A	407	CLA	MG-ND	-3.82	1.98	2.05
28	G	612	CLA	MG-ND	-3.82	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	N	614	CLA	MG-ND	-3.82	1.98	2.05
34	b	620	C7Z	C15-C14	3.81	1.55	1.43
28	S	610	CLA	MG-ND	-3.81	1.98	2.05
28	G	613	CLA	MG-ND	-3.81	1.98	2.05
28	b	610	CLA	MG-ND	-3.81	1.98	2.05
28	c	509	CLA	MG-ND	-3.80	1.98	2.05
28	N	610	CLA	MG-ND	-3.80	1.98	2.05
43	H	101	RRX	C15-C14	3.80	1.55	1.43
28	N	611	CLA	MG-ND	-3.80	1.98	2.05
28	Y	612	CLA	MG-ND	-3.80	1.98	2.05
43	H	101	RRX	C20-C21	3.80	1.55	1.43
28	S	612	CLA	MG-ND	-3.79	1.98	2.05
28	S	602	CLA	MG-ND	-3.79	1.98	2.05
28	N	612	CLA	MG-ND	-3.79	1.98	2.05
28	Y	604	CLA	MG-ND	-3.79	1.98	2.05
28	B	616	CLA	MG-ND	-3.78	1.98	2.05
28	S	609	CLA	MG-ND	-3.78	1.98	2.05
28	G	611	CLA	MG-ND	-3.78	1.98	2.05
28	b	602	CLA	MG-ND	-3.78	1.98	2.05
28	D	403	CLA	MG-ND	-3.78	1.98	2.05
28	Y	614	CLA	MG-ND	-3.78	1.98	2.05
28	C	502	CLA	MG-ND	-3.78	1.98	2.05
28	C	501	CLA	MG-ND	-3.78	1.98	2.05
28	S	604	CLA	MG-ND	-3.77	1.98	2.05
41	D	405	PL9	C7-C3	-3.77	1.47	1.51
28	B	603	CLA	MG-ND	-3.77	1.98	2.05
28	Y	610	CLA	MG-ND	-3.76	1.98	2.05
28	c	503	CLA	MG-ND	-3.76	1.98	2.05
28	c	501	CLA	MG-ND	-3.76	1.98	2.05
28	c	513	CLA	MG-ND	-3.76	1.98	2.05
28	Y	602	CLA	MG-ND	-3.75	1.98	2.05
28	b	606	CLA	MG-ND	-3.75	1.98	2.05
28	B	606	CLA	MG-ND	-3.75	1.98	2.05
28	B	602	CLA	MG-ND	-3.75	1.98	2.05
28	c	511	CLA	MG-ND	-3.75	1.98	2.05
28	C	511	CLA	MG-ND	-3.74	1.98	2.05
28	Y	611	CLA	MG-ND	-3.73	1.98	2.05
28	S	613	CLA	MG-ND	-3.73	1.98	2.05
28	B	614	CLA	MG-ND	-3.73	1.98	2.05
28	d	403	CLA	MG-ND	-3.72	1.98	2.05
28	N	603	CLA	MG-ND	-3.72	1.98	2.05
28	a	405	CLA	MG-ND	-3.71	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	620	C7Z	C27-C26	3.70	1.58	1.45
28	Y	613	CLA	MG-ND	-3.69	1.98	2.05
28	b	616	CLA	MG-ND	-3.69	1.98	2.05
28	G	610	CLA	MG-ND	-3.68	1.98	2.05
28	Y	603	CLA	MG-ND	-3.68	1.98	2.05
34	b	620	C7Z	C27-C26	3.68	1.58	1.45
28	C	504	CLA	MG-ND	-3.68	1.98	2.05
37	b	625	DGA	OG2-CB1	3.67	1.44	1.34
28	N	602	CLA	MG-ND	-3.66	1.98	2.05
28	B	612	CLA	C1C-NC	-3.65	1.32	1.37
28	G	603	CLA	MG-ND	-3.64	1.98	2.05
37	B	625	DGA	OG2-CB1	3.64	1.44	1.34
28	G	614	CLA	MG-ND	-3.64	1.98	2.05
34	b	620	C7Z	C35-C34	3.64	1.54	1.43
28	c	510	CLA	MG-ND	-3.63	1.98	2.05
34	B	620	C7Z	C35-C34	3.60	1.54	1.43
34	b	620	C7Z	C2-C1	3.60	1.66	1.54
28	B	611	CLA	C1C-NC	-3.59	1.32	1.37
28	A	406	CLA	C1C-NC	-3.59	1.32	1.37
34	B	620	C7Z	C2-C1	3.59	1.66	1.54
28	c	508	CLA	C1C-NC	-3.58	1.32	1.37
28	C	508	CLA	C1C-NC	-3.55	1.32	1.37
28	B	605	CLA	C1C-NC	-3.54	1.32	1.37
37	J	101	DGA	OG2-CB1	3.53	1.44	1.34
28	c	504	CLA	C1C-NC	-3.53	1.32	1.37
37	j	101	DGA	OG2-CB1	3.51	1.44	1.34
37	c	524	DGA	OG2-CB1	3.51	1.44	1.34
28	b	611	CLA	C1C-NC	-3.50	1.32	1.37
45	k	101	4RF	O18-C16	3.49	1.43	1.33
42	f	101	HEM	C3C-C2C	-3.49	1.35	1.40
28	b	617	CLA	C1C-NC	-3.48	1.32	1.37
28	c	507	CLA	C1C-NC	-3.48	1.32	1.37
28	G	602	CLA	C1C-NC	-3.47	1.32	1.37
45	i	101	4RF	O18-C16	3.46	1.43	1.33
34	B	620	C7Z	C38-C25	3.46	1.56	1.50
28	C	509	CLA	C1C-NC	-3.45	1.32	1.37
45	K	101	4RF	O18-C16	3.45	1.43	1.33
28	c	506	CLA	C1C-NC	-3.45	1.32	1.37
45	I	102	4RF	O18-C16	3.44	1.43	1.33
43	h	101	RRX	C11-C10	3.44	1.54	1.43
28	B	617	CLA	C1C-NC	-3.44	1.32	1.37
28	b	605	CLA	C1C-NC	-3.44	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	524	DGA	OG2-CB1	3.44	1.44	1.34
42	F	101	HEM	C3C-C2C	-3.43	1.35	1.40
28	C	502	CLA	C1C-NC	-3.43	1.32	1.37
46	N	608	CHL	CBB-CAB	3.42	1.52	1.29
34	b	620	C7Z	C7-C6	3.42	1.57	1.45
28	N	610	CLA	C1C-NC	-3.42	1.32	1.37
28	C	506	CLA	C1C-NC	-3.41	1.32	1.37
34	b	620	C7Z	C38-C25	3.41	1.56	1.50
28	B	610	CLA	C1C-NC	-3.41	1.32	1.37
46	Y	601	CHL	CBB-CAB	3.41	1.51	1.29
28	C	513	CLA	C1C-NC	-3.41	1.32	1.37
28	c	504	CLA	CBB-CAB	3.41	1.51	1.29
46	G	607	CHL	CBB-CAB	3.41	1.51	1.29
37	J	101	DGA	OG1-CA1	3.40	1.43	1.33
28	B	606	CLA	C1C-NC	-3.39	1.32	1.37
46	G	605	CHL	CBB-CAB	3.39	1.51	1.29
28	b	611	CLA	CBB-CAB	3.39	1.51	1.29
28	b	610	CLA	C1C-NC	-3.39	1.32	1.37
28	a	407	CLA	C1C-NC	-3.38	1.32	1.37
28	c	512	CLA	CBB-CAB	3.38	1.51	1.29
28	d	402	CLA	CBB-CAB	3.38	1.51	1.29
43	H	101	RRX	C11-C10	3.38	1.53	1.43
28	c	508	CLA	CBB-CAB	3.38	1.51	1.29
28	S	612	CLA	CBB-CAB	3.38	1.51	1.29
28	B	612	CLA	CBB-CAB	3.38	1.51	1.29
28	S	603	CLA	CBB-CAB	3.38	1.51	1.29
28	G	603	CLA	CBB-CAB	3.38	1.51	1.29
46	Y	605	CHL	CBB-CAB	3.38	1.51	1.29
46	N	601	CHL	CBB-CAB	3.38	1.51	1.29
28	b	612	CLA	CBB-CAB	3.38	1.51	1.29
28	c	509	CLA	CBB-CAB	3.38	1.51	1.29
28	c	513	CLA	CBB-CAB	3.38	1.51	1.29
28	C	508	CLA	CBB-CAB	3.37	1.51	1.29
46	S	608	CHL	CBB-CAB	3.37	1.51	1.29
28	b	608	CLA	CBB-CAB	3.37	1.51	1.29
28	C	509	CLA	CBB-CAB	3.37	1.51	1.29
28	c	511	CLA	CBB-CAB	3.37	1.51	1.29
28	b	614	CLA	CBB-CAB	3.37	1.51	1.29
46	G	601	CHL	CBB-CAB	3.37	1.51	1.29
28	A	405	CLA	CBB-CAB	3.37	1.51	1.29
46	G	608	CHL	CBB-CAB	3.37	1.51	1.29
28	c	507	CLA	CBB-CAB	3.37	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	G	614	CLA	CBB-CAB	3.37	1.51	1.29
28	b	610	CLA	CBB-CAB	3.37	1.51	1.29
28	c	503	CLA	CBB-CAB	3.37	1.51	1.29
28	C	503	CLA	CBB-CAB	3.37	1.51	1.29
28	N	614	CLA	CBB-CAB	3.37	1.51	1.29
28	Y	610	CLA	CBB-CAB	3.37	1.51	1.29
28	c	505	CLA	CBB-CAB	3.37	1.51	1.29
28	a	405	CLA	CBB-CAB	3.37	1.51	1.29
28	B	610	CLA	CBB-CAB	3.37	1.51	1.29
46	N	605	CHL	CBB-CAB	3.36	1.51	1.29
34	B	620	C7Z	C7-C6	3.36	1.57	1.45
28	C	504	CLA	C1C-NC	-3.36	1.32	1.37
28	a	407	CLA	CBB-CAB	3.36	1.51	1.29
28	d	403	CLA	CBB-CAB	3.36	1.51	1.29
28	B	609	CLA	CBB-CAB	3.36	1.51	1.29
28	G	610	CLA	CBB-CAB	3.36	1.51	1.29
28	N	613	CLA	CBB-CAB	3.36	1.51	1.29
28	B	614	CLA	CBB-CAB	3.36	1.51	1.29
28	B	611	CLA	CBB-CAB	3.36	1.51	1.29
28	B	608	CLA	CBB-CAB	3.36	1.51	1.29
46	G	609	CHL	CBB-CAB	3.36	1.51	1.29
28	B	604	CLA	CBB-CAB	3.36	1.51	1.29
28	Y	602	CLA	CBB-CAB	3.36	1.51	1.29
28	S	605	CLA	CBB-CAB	3.36	1.51	1.29
28	S	614	CLA	CBB-CAB	3.36	1.51	1.29
28	B	602	CLA	CBB-CAB	3.36	1.51	1.29
28	C	512	CLA	CBB-CAB	3.36	1.51	1.29
28	b	612	CLA	C1C-NC	-3.36	1.32	1.37
28	B	605	CLA	CBB-CAB	3.36	1.51	1.29
28	G	604	CLA	CBB-CAB	3.36	1.51	1.29
28	b	604	CLA	CBB-CAB	3.36	1.51	1.29
28	S	602	CLA	CBB-CAB	3.36	1.51	1.29
28	Y	604	CLA	CBB-CAB	3.36	1.51	1.29
28	Y	608	CLA	CBB-CAB	3.35	1.51	1.29
28	c	501	CLA	CBB-CAB	3.35	1.51	1.29
28	Y	611	CLA	CBB-CAB	3.35	1.51	1.29
28	C	511	CLA	CBB-CAB	3.35	1.51	1.29
28	S	617	CLA	CBB-CAB	3.35	1.51	1.29
28	S	604	CLA	CBB-CAB	3.35	1.51	1.29
28	B	606	CLA	CBB-CAB	3.35	1.51	1.29
28	N	610	CLA	CBB-CAB	3.35	1.51	1.29
28	C	507	CLA	CBB-CAB	3.35	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	N	612	CLA	CBB-CAB	3.35	1.51	1.29
28	A	405	CLA	C1C-NC	-3.35	1.32	1.37
37	c	524	DGA	OG1-CA1	3.35	1.43	1.33
28	G	611	CLA	CBB-CAB	3.35	1.51	1.29
28	B	615	CLA	CBB-CAB	3.35	1.51	1.29
28	C	502	CLA	CBB-CAB	3.35	1.51	1.29
28	S	610	CLA	CBB-CAB	3.35	1.51	1.29
28	N	602	CLA	CBB-CAB	3.35	1.51	1.29
28	B	603	CLA	CBB-CAB	3.35	1.51	1.29
28	c	502	CLA	CBB-CAB	3.35	1.51	1.29
28	b	609	CLA	CBB-CAB	3.35	1.51	1.29
43	h	101	RRX	C16-C17	3.35	1.53	1.43
28	c	506	CLA	CBB-CAB	3.35	1.51	1.29
28	B	617	CLA	CBB-CAB	3.35	1.51	1.29
28	b	607	CLA	CBB-CAB	3.35	1.51	1.29
37	B	625	DGA	OG1-CA1	3.35	1.43	1.33
28	B	607	CLA	CBB-CAB	3.35	1.51	1.29
28	S	613	CLA	CBB-CAB	3.34	1.51	1.29
28	Y	603	CLA	CBB-CAB	3.34	1.51	1.29
28	Y	613	CLA	CBB-CAB	3.34	1.51	1.29
46	N	607	CHL	CBB-CAB	3.34	1.51	1.29
46	Y	607	CHL	CBB-CAB	3.34	1.51	1.29
28	N	604	CLA	CBB-CAB	3.34	1.51	1.29
28	a	406	CLA	CBB-CAB	3.34	1.51	1.29
46	S	607	CHL	CBB-CAB	3.34	1.51	1.29
28	c	510	CLA	CBB-CAB	3.34	1.51	1.29
28	G	602	CLA	CBB-CAB	3.34	1.51	1.29
46	N	609	CHL	CBB-CAB	3.34	1.51	1.29
28	b	616	CLA	CBB-CAB	3.34	1.51	1.29
28	G	612	CLA	CBB-CAB	3.34	1.51	1.29
28	b	603	CLA	CBB-CAB	3.34	1.51	1.29
28	b	615	CLA	CBB-CAB	3.34	1.51	1.29
28	C	501	CLA	CBB-CAB	3.34	1.51	1.29
28	b	617	CLA	CBB-CAB	3.34	1.51	1.29
28	b	602	CLA	CBB-CAB	3.34	1.51	1.29
28	G	613	CLA	CBB-CAB	3.34	1.51	1.29
28	N	611	CLA	CBB-CAB	3.33	1.51	1.29
28	b	613	CLA	CBB-CAB	3.33	1.51	1.29
28	C	505	CLA	CBB-CAB	3.33	1.51	1.29
37	j	101	DGA	OG1-CA1	3.33	1.43	1.33
28	b	606	CLA	CBB-CAB	3.33	1.51	1.29
28	Y	612	CLA	CBB-CAB	3.33	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	407	CLA	CBB-CAB	3.33	1.51	1.29
28	D	402	CLA	CBB-CAB	3.33	1.51	1.29
28	S	609	CLA	CBB-CAB	3.33	1.51	1.29
46	Y	609	CHL	CBB-CAB	3.33	1.51	1.29
28	B	616	CLA	CBB-CAB	3.33	1.51	1.29
28	C	506	CLA	CBB-CAB	3.33	1.51	1.29
28	C	504	CLA	CBB-CAB	3.33	1.51	1.29
28	N	603	CLA	CBB-CAB	3.33	1.51	1.29
28	S	611	CLA	CBB-CAB	3.33	1.51	1.29
28	B	613	CLA	CBB-CAB	3.32	1.51	1.29
28	b	605	CLA	CBB-CAB	3.32	1.51	1.29
28	Y	614	CLA	CBB-CAB	3.32	1.51	1.29
46	S	601	CHL	C4B-NB	3.31	1.38	1.35
28	c	509	CLA	C1C-NC	-3.31	1.32	1.37
28	C	513	CLA	CBB-CAB	3.31	1.51	1.29
28	C	510	CLA	CBB-CAB	3.31	1.51	1.29
28	c	502	CLA	C1C-NC	-3.31	1.32	1.37
46	N	606	CHL	C4B-NB	3.30	1.38	1.35
28	D	403	CLA	C1C-NC	-3.30	1.32	1.37
28	A	406	CLA	CBB-CAB	3.30	1.51	1.29
28	D	402	CLA	C1C-NC	-3.30	1.32	1.37
28	a	405	CLA	C1C-NC	-3.30	1.32	1.37
37	C	524	DGA	OG1-CA1	3.29	1.43	1.33
46	S	601	CHL	CBB-CAB	3.29	1.51	1.29
28	d	402	CLA	C1C-NC	-3.29	1.32	1.37
28	b	606	CLA	C1C-NC	-3.29	1.32	1.37
28	D	403	CLA	CBB-CAB	3.29	1.51	1.29
46	Y	606	CHL	CBB-CAB	3.29	1.51	1.29
28	B	613	CLA	C1C-NC	-3.29	1.32	1.37
28	G	603	CLA	C1C-NC	-3.29	1.32	1.37
32	H	102	LMG	C37-C36	-3.28	1.33	1.51
28	S	610	CLA	C1C-NC	-3.28	1.32	1.37
28	G	612	CLA	C1C-NC	-3.28	1.32	1.37
46	G	608	CHL	C4B-NB	3.28	1.38	1.35
28	S	604	CLA	C1C-NC	-3.28	1.32	1.37
28	S	605	CLA	C1C-NC	-3.28	1.32	1.37
35	c	519	DGD	CAB-C9B	-3.28	1.33	1.51
28	G	611	CLA	C1C-NC	-3.28	1.32	1.37
37	b	625	DGA	OG1-CA1	3.28	1.42	1.33
28	N	604	CLA	C1C-NC	-3.27	1.32	1.37
46	G	606	CHL	CBB-CAB	3.27	1.51	1.29
32	h	102	LMG	C19-C18	-3.27	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	519	DGD	CAB-C9B	-3.27	1.33	1.51
28	B	608	CLA	C1C-NC	-3.27	1.32	1.37
46	Y	606	CHL	C4B-NB	3.26	1.38	1.35
28	A	407	CLA	C1C-NC	-3.26	1.32	1.37
43	h	101	RRX	C29-C30	3.26	1.65	1.54
28	C	507	CLA	C1C-NC	-3.26	1.32	1.37
32	b	622	LMG	C22-C21	-3.26	1.33	1.51
32	c	521	LMG	C22-C21	-3.26	1.33	1.51
43	H	101	RRX	C29-C30	3.26	1.65	1.54
28	a	406	CLA	C1C-NC	-3.26	1.32	1.37
32	B	622	LMG	C22-C21	-3.25	1.33	1.51
28	S	603	CLA	C1C-NC	-3.25	1.33	1.37
28	A	410	CLA	CBB-CAB	3.25	1.50	1.29
46	G	606	CHL	C4B-NB	3.25	1.38	1.35
43	H	101	RRX	C16-C17	3.25	1.53	1.43
35	c	519	DGD	CDA-CCA	-3.25	1.33	1.51
32	H	102	LMG	C19-C18	-3.24	1.33	1.51
28	S	613	CLA	C1C-NC	-3.24	1.33	1.37
35	C	520	DGD	CAB-C9B	-3.24	1.33	1.51
35	c	520	DGD	CAB-C9B	-3.24	1.33	1.51
28	b	616	CLA	C1C-NC	-3.24	1.33	1.37
35	c	518	DGD	CDB-CCB	-3.24	1.33	1.51
46	Y	605	CHL	C4B-NB	3.24	1.38	1.35
43	h	101	RRX	C24-C25	3.24	1.56	1.45
35	C	519	DGD	CDA-CCA	-3.24	1.33	1.51
28	Y	602	CLA	C1C-NC	-3.24	1.33	1.37
28	N	602	CLA	C1C-NC	-3.23	1.33	1.37
32	c	521	LMG	C40-C39	-3.23	1.33	1.51
28	Y	603	CLA	C1C-NC	-3.23	1.33	1.37
32	C	521	LMG	C40-C39	-3.23	1.33	1.51
32	C	521	LMG	C22-C21	-3.23	1.33	1.51
28	S	614	CLA	C1C-NC	-3.23	1.33	1.37
35	c	520	DGD	CAA-C9A	-3.23	1.33	1.51
32	c	523	LMG	C40-C39	-3.23	1.33	1.51
35	C	518	DGD	CDB-CCB	-3.23	1.33	1.51
28	Y	610	CLA	C1C-NC	-3.23	1.33	1.37
46	N	606	CHL	CBB-CAB	3.23	1.50	1.29
32	C	523	LMG	C40-C39	-3.23	1.33	1.51
28	G	610	CLA	C1C-NC	-3.23	1.33	1.37
32	C	523	LMG	C25-C24	-3.23	1.33	1.51
32	c	523	LMG	C25-C24	-3.23	1.33	1.51
32	c	521	LMG	C37-C36	-3.23	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	523	LMG	C37-C36	-3.23	1.33	1.51
32	c	523	LMG	C37-C36	-3.22	1.33	1.51
28	N	611	CLA	C1C-NC	-3.22	1.33	1.37
28	b	608	CLA	C1C-NC	-3.22	1.33	1.37
28	c	505	CLA	C1C-NC	-3.22	1.33	1.37
32	C	523	LMG	C22-C21	-3.22	1.33	1.51
32	W	201	LMG	C40-C39	-3.22	1.33	1.51
32	h	102	LMG	C37-C36	-3.22	1.33	1.51
35	c	520	DGD	CDB-CCB	-3.22	1.33	1.51
28	a	410	CLA	CBB-CAB	3.22	1.50	1.29
28	C	503	CLA	C1C-NC	-3.22	1.33	1.37
32	a	413	LMG	C19-C18	-3.22	1.33	1.51
46	S	608	CHL	C4B-NB	3.22	1.38	1.35
46	Y	609	CHL	C4B-NB	3.22	1.38	1.35
35	C	520	DGD	CAA-C9A	-3.22	1.33	1.51
32	c	523	LMG	C22-C21	-3.22	1.33	1.51
32	A	413	LMG	C40-C39	-3.22	1.33	1.51
28	C	510	CLA	C1C-NC	-3.22	1.33	1.37
28	b	613	CLA	C1C-NC	-3.22	1.33	1.37
32	a	413	LMG	C37-C36	-3.21	1.33	1.51
28	G	604	CLA	C1C-NC	-3.21	1.33	1.37
28	c	510	CLA	C1C-NC	-3.21	1.33	1.37
35	c	519	DGD	CAA-C9A	-3.21	1.33	1.51
35	C	519	DGD	CDB-CCB	-3.21	1.33	1.51
32	D	411	LMG	C22-C21	-3.21	1.33	1.51
28	Y	612	CLA	C1C-NC	-3.21	1.33	1.37
46	S	606	CHL	C4B-NB	3.21	1.38	1.35
35	C	518	DGD	CAB-C9B	-3.21	1.33	1.51
35	C	519	DGD	CAA-C9A	-3.21	1.33	1.51
46	S	607	CHL	C4B-NB	3.21	1.38	1.35
32	A	413	LMG	C37-C36	-3.21	1.33	1.51
32	H	102	LMG	C40-C39	-3.21	1.33	1.51
28	c	503	CLA	C1C-NC	-3.21	1.33	1.37
28	C	505	CLA	C1C-NC	-3.20	1.33	1.37
46	S	606	CHL	CBB-CAB	3.20	1.50	1.29
32	b	622	LMG	C19-C18	-3.20	1.33	1.51
28	B	614	CLA	C1C-NC	-3.20	1.33	1.37
28	N	612	CLA	C1C-NC	-3.20	1.33	1.37
28	b	602	CLA	C1C-NC	-3.20	1.33	1.37
35	c	519	DGD	CDB-CCB	-3.20	1.33	1.51
46	N	605	CHL	C4B-NB	3.20	1.38	1.35
46	G	605	CHL	C4B-NB	3.20	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	614	CLA	C1C-NC	-3.20	1.33	1.37
28	B	607	CLA	C1C-NC	-3.20	1.33	1.37
28	A	410	CLA	C1C-NC	-3.20	1.33	1.37
28	N	614	CLA	C1C-NC	-3.20	1.33	1.37
32	A	413	LMG	C19-C18	-3.20	1.33	1.51
35	c	518	DGD	CAB-C9B	-3.20	1.33	1.51
28	Y	614	CLA	C1C-NC	-3.20	1.33	1.37
32	C	523	LMG	C43-C42	-3.20	1.33	1.51
32	D	411	LMG	C19-C18	-3.20	1.33	1.51
32	a	413	LMG	C40-C39	-3.19	1.33	1.51
32	C	521	LMG	C19-C18	-3.19	1.33	1.51
32	d	411	LMG	C22-C21	-3.19	1.33	1.51
28	S	612	CLA	C1C-NC	-3.19	1.33	1.37
32	w	201	LMG	C37-C36	-3.19	1.33	1.51
28	B	616	CLA	C1C-NC	-3.19	1.33	1.37
32	W	201	LMG	C37-C36	-3.19	1.33	1.51
32	B	622	LMG	C19-C18	-3.19	1.33	1.51
28	N	613	CLA	C1C-NC	-3.19	1.33	1.37
32	C	521	LMG	C37-C36	-3.19	1.33	1.51
32	h	102	LMG	C40-C39	-3.19	1.33	1.51
32	c	523	LMG	C43-C42	-3.19	1.33	1.51
28	S	611	CLA	C1C-NC	-3.19	1.33	1.37
28	b	604	CLA	C1C-NC	-3.19	1.33	1.37
32	c	523	LMG	C19-C18	-3.19	1.33	1.51
28	S	617	CLA	C1C-NC	-3.18	1.33	1.37
32	d	411	LMG	C19-C18	-3.18	1.33	1.51
35	C	520	DGD	CDB-CCB	-3.18	1.33	1.51
28	S	602	CLA	C1C-NC	-3.18	1.33	1.37
28	B	603	CLA	C1C-NC	-3.18	1.33	1.37
28	B	602	CLA	C1C-NC	-3.18	1.33	1.37
28	b	609	CLA	C1C-NC	-3.18	1.33	1.37
43	H	101	RRX	C24-C25	3.17	1.56	1.45
28	c	513	CLA	C1C-NC	-3.17	1.33	1.37
28	B	604	CLA	C1C-NC	-3.17	1.33	1.37
28	N	603	CLA	C1C-NC	-3.17	1.33	1.37
28	b	603	CLA	C1C-NC	-3.16	1.33	1.37
28	b	615	CLA	C1C-NC	-3.16	1.33	1.37
32	c	521	LMG	C19-C18	-3.16	1.33	1.51
28	G	614	CLA	C1C-NC	-3.16	1.33	1.37
28	C	501	CLA	C1C-NC	-3.16	1.33	1.37
28	a	410	CLA	C1C-NC	-3.16	1.33	1.37
28	Y	604	CLA	C1C-NC	-3.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	512	CLA	C1C-NC	-3.16	1.33	1.37
28	S	609	CLA	C1C-NC	-3.15	1.33	1.37
42	F	101	HEM	CAB-C3B	3.15	1.56	1.47
28	G	613	CLA	C1C-NC	-3.15	1.33	1.37
28	Y	613	CLA	C1C-NC	-3.15	1.33	1.37
32	C	523	LMG	C19-C18	-3.15	1.33	1.51
32	w	201	LMG	C40-C39	-3.14	1.33	1.51
28	B	615	CLA	C1C-NC	-3.14	1.33	1.37
28	B	609	CLA	C1C-NC	-3.14	1.33	1.37
28	C	512	CLA	C1C-NC	-3.14	1.33	1.37
28	c	511	CLA	C1C-NC	-3.14	1.33	1.37
42	f	101	HEM	CAB-C3B	3.13	1.56	1.47
28	b	607	CLA	C1C-NC	-3.12	1.33	1.37
28	c	501	CLA	C1C-NC	-3.12	1.33	1.37
46	G	601	CHL	C4B-NB	3.12	1.38	1.35
28	d	403	CLA	C1C-NC	-3.11	1.33	1.37
28	C	511	CLA	C1C-NC	-3.11	1.33	1.37
28	Y	611	CLA	C1C-NC	-3.10	1.33	1.37
45	K	101	4RF	O40-C41	3.09	1.42	1.33
45	I	102	4RF	O40-C41	3.08	1.42	1.33
43	H	101	RRX	C4-C5	-3.07	1.44	1.51
46	N	601	CHL	C4B-NB	3.07	1.37	1.35
46	G	609	CHL	C4B-NB	3.07	1.37	1.35
45	i	101	4RF	O40-C41	3.06	1.42	1.33
46	N	608	CHL	C4B-NB	3.05	1.37	1.35
28	Y	608	CLA	C1C-NC	-3.05	1.33	1.37
43	h	101	RRX	C7-C6	3.03	1.55	1.45
41	D	405	PL9	C3-C4	-3.02	1.44	1.49
45	k	101	4RF	O40-C41	2.98	1.42	1.33
46	S	606	CHL	C3B-C2B	-2.98	1.36	1.40
46	Y	601	CHL	C4B-NB	2.98	1.37	1.35
46	Y	607	CHL	C4B-NB	2.97	1.37	1.35
43	h	101	RRX	C4-C5	-2.95	1.45	1.51
43	H	101	RRX	C7-C6	2.93	1.55	1.45
46	N	607	CHL	C4B-NB	2.90	1.37	1.35
50	S	625	LPX	P1-O1	2.86	1.70	1.59
43	h	101	RRX	C32-C1	2.85	1.59	1.53
46	G	606	CHL	C3B-C2B	-2.84	1.36	1.40
45	k	101	4RF	O21-C22	2.84	1.42	1.34
46	G	607	CHL	C4B-NB	2.82	1.37	1.35
46	N	609	CHL	C4B-NB	2.80	1.37	1.35
28	D	402	CLA	CHC-C1C	2.78	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	501	CLA	CHC-C1C	2.78	1.42	1.35
45	K	101	4RF	O21-C22	2.77	1.42	1.34
43	H	101	RRX	C32-C1	2.76	1.59	1.53
28	S	610	CLA	CHC-C1C	2.76	1.42	1.35
29	a	408	PHO	CAC-C3C	-2.75	1.47	1.52
28	c	503	CLA	CHC-C1C	2.74	1.42	1.35
28	c	508	CLA	CHC-C1C	2.74	1.42	1.35
34	b	620	C7Z	C21-C26	-2.73	1.50	1.53
28	G	610	CLA	CHC-C1C	2.72	1.41	1.35
45	I	102	4RF	O21-C22	2.72	1.42	1.34
28	Y	602	CLA	CHC-C1C	2.71	1.41	1.35
28	c	513	CLA	CHC-C1C	2.71	1.41	1.35
28	C	501	CLA	CHC-C1C	2.70	1.41	1.35
41	d	405	PL9	C3-C4	-2.70	1.45	1.49
28	Y	610	CLA	CHC-C1C	2.70	1.41	1.35
28	Y	613	CLA	CHC-C1C	2.70	1.41	1.35
28	b	613	CLA	CHC-C1C	2.70	1.41	1.35
45	i	101	4RF	O21-C22	2.70	1.41	1.34
34	B	620	C7Z	C21-C26	-2.70	1.50	1.53
29	A	409	PHO	CAC-C3C	-2.70	1.47	1.52
28	b	615	CLA	CHC-C1C	2.70	1.41	1.35
28	S	602	CLA	CHC-C1C	2.69	1.41	1.35
28	C	505	CLA	CHC-C1C	2.68	1.41	1.35
28	b	612	CLA	CHC-C1C	2.68	1.41	1.35
28	N	602	CLA	CHC-C1C	2.68	1.41	1.35
28	C	508	CLA	CHC-C1C	2.68	1.41	1.35
28	S	611	CLA	C3B-C2B	-2.67	1.36	1.40
28	b	610	CLA	CHC-C1C	2.67	1.41	1.35
28	B	616	CLA	CHC-C1C	2.66	1.41	1.35
28	C	503	CLA	CHC-C1C	2.66	1.41	1.35
28	a	405	CLA	CHC-C1C	2.66	1.41	1.35
28	d	402	CLA	CHC-C1C	2.66	1.41	1.35
28	d	403	CLA	CHC-C1C	2.66	1.41	1.35
28	G	614	CLA	CHC-C1C	2.66	1.41	1.35
28	S	612	CLA	CHC-C1C	2.66	1.41	1.35
28	a	410	CLA	CHC-C1C	2.65	1.41	1.35
28	S	613	CLA	CHC-C1C	2.65	1.41	1.35
28	G	613	CLA	CHC-C1C	2.64	1.41	1.35
28	C	504	CLA	CHC-C1C	2.64	1.41	1.35
28	b	608	CLA	CHC-C1C	2.64	1.41	1.35
28	G	604	CLA	CHC-C1C	2.64	1.41	1.35
28	Y	604	CLA	CHC-C1C	2.64	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y	611	CLA	CHC-C1C	2.64	1.41	1.35
28	N	614	CLA	CHC-C1C	2.64	1.41	1.35
28	B	616	CLA	C3B-C2B	-2.63	1.36	1.40
28	B	607	CLA	CHC-C1C	2.63	1.41	1.35
28	N	612	CLA	CHC-C1C	2.63	1.41	1.35
28	b	603	CLA	CHC-C1C	2.63	1.41	1.35
28	B	603	CLA	CHC-C1C	2.62	1.41	1.35
28	c	504	CLA	C3B-C2B	-2.62	1.36	1.40
28	S	609	CLA	CHC-C1C	2.62	1.41	1.35
28	B	604	CLA	CHC-C1C	2.62	1.41	1.35
28	c	507	CLA	C3B-C2B	-2.62	1.36	1.40
28	A	410	CLA	CHC-C1C	2.62	1.41	1.35
28	S	614	CLA	CHC-C1C	2.61	1.41	1.35
28	N	603	CLA	CHC-C1C	2.61	1.41	1.35
28	b	602	CLA	CHC-C1C	2.61	1.41	1.35
28	b	616	CLA	CHC-C1C	2.61	1.41	1.35
28	B	615	CLA	CHC-C1C	2.61	1.41	1.35
28	N	613	CLA	CHC-C1C	2.61	1.41	1.35
28	C	512	CLA	CHC-C1C	2.61	1.41	1.35
28	C	504	CLA	C3B-C2B	-2.61	1.36	1.40
28	Y	614	CLA	CHC-C1C	2.61	1.41	1.35
28	C	513	CLA	CHC-C1C	2.61	1.41	1.35
28	b	607	CLA	CHC-C1C	2.61	1.41	1.35
28	A	405	CLA	CHC-C1C	2.60	1.41	1.35
28	A	407	CLA	CHC-C1C	2.60	1.41	1.35
28	S	605	CLA	CHC-C1C	2.60	1.41	1.35
28	c	511	CLA	CHC-C1C	2.60	1.41	1.35
28	Y	603	CLA	CHC-C1C	2.60	1.41	1.35
28	Y	608	CLA	CHC-C1C	2.59	1.41	1.35
28	S	617	CLA	CHC-C1C	2.59	1.41	1.35
28	B	602	CLA	CHC-C1C	2.59	1.41	1.35
28	c	506	CLA	C3B-C2B	-2.59	1.36	1.40
28	D	403	CLA	C3B-C2B	-2.59	1.36	1.40
28	b	609	CLA	CHC-C1C	2.59	1.41	1.35
28	N	604	CLA	CHC-C1C	2.59	1.41	1.35
28	C	511	CLA	CHC-C1C	2.59	1.41	1.35
28	G	612	CLA	CHC-C1C	2.58	1.41	1.35
28	D	403	CLA	CHC-C1C	2.58	1.41	1.35
28	c	512	CLA	CHC-C1C	2.58	1.41	1.35
28	b	604	CLA	CHC-C1C	2.58	1.41	1.35
46	N	606	CHL	C3B-C2B	-2.58	1.36	1.40
28	c	505	CLA	CHC-C1C	2.58	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	411	LMG	C37-C36	-2.57	1.33	1.51
28	B	609	CLA	CHC-C1C	2.57	1.41	1.35
28	B	614	CLA	CHC-C1C	2.57	1.41	1.35
28	B	610	CLA	CHC-C1C	2.56	1.41	1.35
28	Y	612	CLA	CHC-C1C	2.56	1.41	1.35
32	D	411	LMG	C37-C36	-2.56	1.33	1.51
28	Y	603	CLA	C3B-C2B	-2.56	1.36	1.40
28	B	608	CLA	CHC-C1C	2.56	1.41	1.35
28	B	612	CLA	CHC-C1C	2.56	1.41	1.35
28	N	611	CLA	CHC-C1C	2.55	1.41	1.35
28	G	611	CLA	CHC-C1C	2.55	1.41	1.35
28	G	603	CLA	C3B-C2B	-2.55	1.36	1.40
28	b	614	CLA	CHC-C1C	2.55	1.41	1.35
28	c	510	CLA	CHC-C1C	2.55	1.41	1.35
28	C	506	CLA	C3B-C2B	-2.55	1.36	1.40
28	C	510	CLA	C3B-C2B	-2.54	1.36	1.40
36	b	624	3PH	O21-C2	-2.54	1.40	1.46
28	b	616	CLA	C3B-C2B	-2.54	1.36	1.40
28	a	406	CLA	CHC-C1C	2.54	1.41	1.35
28	b	605	CLA	C3B-C2B	-2.54	1.36	1.40
28	N	610	CLA	CHC-C1C	2.54	1.41	1.35
28	N	603	CLA	C3B-C2B	-2.54	1.36	1.40
28	a	407	CLA	CHC-C1C	2.54	1.41	1.35
29	A	408	PHO	CAC-C3C	-2.54	1.47	1.52
51	Y	627	PTY	O7-C6	-2.53	1.40	1.46
28	b	617	CLA	CHC-C1C	2.53	1.41	1.35
28	b	606	CLA	CHC-C1C	2.52	1.41	1.35
28	G	602	CLA	CHC-C1C	2.52	1.41	1.35
28	c	510	CLA	C3B-C2B	-2.51	1.36	1.40
28	b	611	CLA	CHC-C1C	2.51	1.41	1.35
28	B	602	CLA	C3B-C2B	-2.50	1.36	1.40
28	C	502	CLA	CHC-C1C	2.50	1.41	1.35
28	b	604	CLA	C3B-C2B	-2.50	1.36	1.40
28	B	613	CLA	CHC-C1C	2.49	1.41	1.35
28	N	611	CLA	C3B-C2B	-2.49	1.36	1.40
28	C	501	CLA	C3B-C2B	-2.49	1.36	1.40
28	Y	612	CLA	C3B-C2B	-2.49	1.36	1.40
28	S	611	CLA	CHC-C1C	2.49	1.41	1.35
28	b	613	CLA	C3B-C2B	-2.48	1.36	1.40
28	C	507	CLA	CHC-C1C	2.48	1.41	1.35
28	B	606	CLA	CHC-C1C	2.48	1.41	1.35
34	b	620	C7Z	C20-C13	2.48	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	t	101	3PH	O21-C2	-2.48	1.40	1.46
28	S	610	CLA	C3B-C2B	-2.47	1.36	1.40
28	B	610	CLA	C3B-C2B	-2.47	1.36	1.40
28	Y	614	CLA	C3B-C2B	-2.47	1.36	1.40
28	S	603	CLA	CHC-C1C	2.47	1.41	1.35
28	c	509	CLA	CHC-C1C	2.47	1.41	1.35
36	S	626	3PH	O21-C2	-2.47	1.40	1.46
28	B	617	CLA	CHC-C1C	2.46	1.41	1.35
28	S	604	CLA	CHC-C1C	2.46	1.41	1.35
28	N	612	CLA	C3B-C2B	-2.46	1.37	1.40
28	B	611	CLA	CHC-C1C	2.46	1.41	1.35
28	b	605	CLA	CHC-C1C	2.45	1.41	1.35
28	S	609	CLA	C3B-C2B	-2.45	1.37	1.40
36	B	624	3PH	O21-C2	-2.45	1.40	1.46
28	S	604	CLA	C3B-C2B	-2.45	1.37	1.40
28	a	407	CLA	C3B-C2B	-2.45	1.37	1.40
28	c	502	CLA	CHC-C1C	2.44	1.41	1.35
28	c	506	CLA	CHC-C1C	2.44	1.41	1.35
28	G	612	CLA	C3B-C2B	-2.44	1.37	1.40
28	C	509	CLA	CHC-C1C	2.44	1.41	1.35
36	b	624	3PH	O31-C31	2.44	1.40	1.33
28	C	510	CLA	CHC-C1C	2.44	1.41	1.35
36	S	626	3PH	O31-C31	2.43	1.40	1.33
51	Y	626	PTY	O7-C6	-2.43	1.40	1.46
51	Y	626	PTY	O4-C30	2.42	1.40	1.33
48	G	622	XAT	O24-C25	-2.42	1.42	1.46
28	S	603	CLA	C3B-C2B	-2.42	1.37	1.40
28	c	501	CLA	C3B-C2B	-2.42	1.37	1.40
43	H	101	RRX	C35-C13	2.42	1.55	1.50
28	C	505	CLA	C3B-C2B	-2.41	1.37	1.40
43	h	101	RRX	C35-C13	2.41	1.55	1.50
36	B	624	3PH	O31-C31	2.40	1.40	1.33
28	G	603	CLA	CHC-C1C	2.40	1.41	1.35
36	T	101	3PH	O31-C31	2.40	1.40	1.33
28	B	611	CLA	C3B-C2B	-2.40	1.37	1.40
34	B	620	C7Z	C18-C5	2.39	1.54	1.50
36	T	101	3PH	O21-C21	2.39	1.41	1.34
36	t	101	3PH	O31-C31	2.39	1.40	1.33
28	C	506	CLA	CHC-C1C	2.38	1.41	1.35
28	D	402	CLA	C3B-C2B	-2.38	1.37	1.40
28	d	403	CLA	C3B-C2B	-2.38	1.37	1.40
28	b	602	CLA	C3B-C2B	-2.38	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	G	613	CLA	C3B-C2B	-2.37	1.37	1.40
28	G	602	CLA	C1C-C2C	2.37	1.49	1.44
28	C	502	CLA	C3B-C2B	-2.36	1.37	1.40
28	b	603	CLA	C3B-C2B	-2.36	1.37	1.40
28	b	611	CLA	C1C-C2C	2.36	1.49	1.44
28	N	614	CLA	C3B-C2B	-2.36	1.37	1.40
28	A	406	CLA	CHC-C1C	2.35	1.41	1.35
28	B	605	CLA	CHC-C1C	2.35	1.41	1.35
28	G	604	CLA	C3B-C2B	-2.35	1.37	1.40
34	b	620	C7Z	C18-C5	2.35	1.54	1.50
28	B	604	CLA	C3B-C2B	-2.35	1.37	1.40
28	B	608	CLA	C3B-C2B	-2.34	1.37	1.40
28	G	611	CLA	C3B-C2B	-2.34	1.37	1.40
28	B	603	CLA	C3B-C2B	-2.34	1.37	1.40
28	N	613	CLA	C3B-C2B	-2.34	1.37	1.40
28	N	610	CLA	C3B-C2B	-2.34	1.37	1.40
28	S	613	CLA	C3B-C2B	-2.33	1.37	1.40
28	S	605	CLA	C3B-C2B	-2.33	1.37	1.40
50	S	625	LPX	P1-O2	2.32	1.68	1.59
29	a	409	PHO	CAC-C3C	-2.32	1.48	1.52
28	B	605	CLA	C1A-CHA	2.32	1.52	1.43
28	b	607	CLA	C3B-C2B	-2.32	1.37	1.40
28	S	603	CLA	C1A-CHA	2.31	1.52	1.43
51	Y	627	PTY	O7-C8	2.31	1.40	1.35
28	S	611	CLA	C1A-CHA	2.31	1.52	1.43
30	B	618	BCR	C1-C6	-2.31	1.50	1.53
28	B	602	CLA	C1A-CHA	2.31	1.52	1.43
28	B	617	CLA	C3B-C2B	-2.31	1.37	1.40
46	Y	609	CHL	C3B-C2B	-2.30	1.37	1.40
28	b	606	CLA	C3B-C2B	-2.30	1.37	1.40
34	B	620	C7Z	C20-C13	2.30	1.55	1.50
28	Y	608	CLA	C3B-C2B	-2.30	1.37	1.40
28	b	614	CLA	C1A-CHA	2.29	1.52	1.43
41	D	405	PL9	C6-C1	-2.29	1.44	1.48
28	A	407	CLA	C3B-C2B	-2.29	1.37	1.40
28	S	614	CLA	C3B-C2B	-2.28	1.37	1.40
28	S	617	CLA	C3B-C2B	-2.28	1.37	1.40
28	c	507	CLA	CHC-C1C	2.28	1.40	1.35
28	c	504	CLA	CHC-C1C	2.28	1.40	1.35
28	C	512	CLA	C1A-CHA	2.27	1.52	1.43
28	c	512	CLA	C1A-CHA	2.27	1.52	1.43
28	N	611	CLA	C1A-CHA	2.26	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	G	609	CHL	C3B-C2B	-2.26	1.37	1.40
28	B	606	CLA	C3B-C2B	-2.26	1.37	1.40
28	b	611	CLA	C3B-C2B	-2.26	1.37	1.40
28	a	407	CLA	C1A-CHA	2.25	1.52	1.43
28	Y	604	CLA	C3B-C2B	-2.25	1.37	1.40
28	G	613	CLA	C1C-C2C	2.25	1.48	1.44
28	b	613	CLA	C1C-C2C	2.25	1.48	1.44
51	Y	626	PTY	O7-C8	2.24	1.40	1.34
28	c	501	CLA	C1C-C2C	2.24	1.48	1.44
28	N	610	CLA	C1A-CHA	2.24	1.52	1.43
28	S	605	CLA	C1A-CHA	2.24	1.52	1.43
28	d	402	CLA	C1C-C2C	2.24	1.48	1.44
28	N	604	CLA	C3B-C2B	-2.24	1.37	1.40
28	C	513	CLA	C1C-C2C	2.24	1.48	1.44
28	A	406	CLA	C1A-CHA	2.24	1.52	1.43
28	B	616	CLA	C1A-CHA	2.23	1.52	1.43
48	Y	622	XAT	O24-C25	-2.23	1.43	1.46
28	b	609	CLA	C1A-CHA	2.23	1.52	1.43
36	t	101	3PH	O21-C21	2.23	1.40	1.34
28	b	605	CLA	C1A-CHA	2.22	1.52	1.43
46	Y	606	CHL	C3B-C2B	-2.22	1.37	1.40
28	N	613	CLA	C1A-CHA	2.22	1.52	1.43
28	c	501	CLA	C1A-CHA	2.22	1.52	1.43
28	b	615	CLA	C1C-C2C	2.22	1.48	1.44
28	S	613	CLA	C1A-CHA	2.22	1.52	1.43
28	a	406	CLA	C1A-CHA	2.22	1.52	1.43
28	c	511	CLA	C1A-CHA	2.22	1.52	1.43
28	S	617	CLA	C1A-CHA	2.22	1.52	1.43
28	S	609	CLA	C1A-CHA	2.21	1.52	1.43
41	d	405	PL9	C53-C6	-2.21	1.46	1.50
28	C	512	CLA	C1C-C2C	2.21	1.48	1.44
28	B	608	CLA	C1A-CHA	2.21	1.52	1.43
28	Y	608	CLA	C1A-CHA	2.21	1.52	1.43
28	c	503	CLA	C1C-C2C	2.21	1.48	1.44
28	C	513	CLA	C1A-CHA	2.20	1.52	1.43
28	b	608	CLA	C1A-CHA	2.20	1.52	1.43
28	Y	611	CLA	C1A-CHA	2.20	1.52	1.43
28	c	505	CLA	C1A-CHA	2.20	1.52	1.43
28	b	603	CLA	C1C-C2C	2.20	1.48	1.44
28	c	504	CLA	C1A-CHA	2.20	1.52	1.43
28	N	614	CLA	C1C-C2C	2.20	1.48	1.44
34	b	620	C7Z	C40-C33	2.20	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	609	CLA	C1B-NB	2.20	1.37	1.35
28	N	603	CLA	C1A-CHA	2.20	1.52	1.43
28	A	407	CLA	C1A-CHA	2.20	1.52	1.43
48	N	622	XAT	O24-C25	-2.20	1.43	1.46
28	B	613	CLA	C3B-C2B	-2.20	1.37	1.40
28	Y	613	CLA	C1A-CHA	2.19	1.52	1.43
28	G	613	CLA	C1A-CHA	2.19	1.52	1.43
28	N	604	CLA	C1A-CHA	2.19	1.52	1.43
28	B	614	CLA	C1A-CHA	2.19	1.52	1.43
28	Y	612	CLA	C1A-CHA	2.19	1.52	1.43
28	c	513	CLA	C1A-CHA	2.19	1.52	1.43
28	N	614	CLA	C1A-CHA	2.19	1.52	1.43
28	C	513	CLA	C3B-C2B	-2.19	1.37	1.40
28	b	602	CLA	C1A-CHA	2.19	1.52	1.43
28	C	503	CLA	C1C-C2C	2.18	1.48	1.44
28	S	604	CLA	C1A-CHA	2.18	1.52	1.43
28	b	616	CLA	C1A-CHA	2.18	1.52	1.43
28	S	612	CLA	C1C-C2C	2.18	1.48	1.44
28	C	505	CLA	C1A-CHA	2.18	1.52	1.43
28	N	613	CLA	C1C-C2C	2.18	1.48	1.44
28	G	613	CLA	C1B-NB	2.18	1.37	1.35
28	B	603	CLA	C1A-CHA	2.18	1.52	1.43
28	C	503	CLA	C1A-CHA	2.18	1.52	1.43
28	S	612	CLA	C1A-CHA	2.18	1.52	1.43
28	N	612	CLA	C1A-CHA	2.17	1.52	1.43
28	C	504	CLA	C1A-CHA	2.17	1.52	1.43
28	d	403	CLA	C1A-CHA	2.17	1.52	1.43
28	G	602	CLA	C3B-C2B	-2.17	1.37	1.40
28	G	610	CLA	C1C-C2C	2.17	1.48	1.44
28	a	410	CLA	C1C-C2C	2.17	1.48	1.44
49	S	623	NEX	C1-C6	-2.17	1.50	1.54
28	b	606	CLA	C1A-CHA	2.17	1.52	1.43
28	b	609	CLA	C1C-C2C	2.17	1.48	1.44
28	B	611	CLA	C1C-C2C	2.16	1.48	1.44
28	c	513	CLA	C1C-C2C	2.16	1.48	1.44
28	b	607	CLA	C1A-CHA	2.16	1.52	1.43
34	B	620	C7Z	C40-C33	2.16	1.55	1.50
28	C	501	CLA	C1C-C2C	2.16	1.48	1.44
28	G	612	CLA	C1A-CHA	2.16	1.52	1.43
28	Y	608	CLA	C1C-C2C	2.16	1.48	1.44
28	G	614	CLA	C1A-CHA	2.16	1.52	1.43
28	G	611	CLA	C1A-CHA	2.16	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	617	CLA	C1A-CHA	2.16	1.52	1.43
28	Y	614	CLA	C1A-CHA	2.16	1.52	1.43
28	G	603	CLA	C1A-CHA	2.16	1.52	1.43
28	B	602	CLA	C1C-C2C	2.16	1.48	1.44
36	B	624	3PH	O21-C21	2.16	1.40	1.34
28	Y	613	CLA	C1C-C2C	2.15	1.48	1.44
28	c	502	CLA	C1A-CHA	2.15	1.52	1.43
28	S	613	CLA	C1B-NB	2.15	1.37	1.35
28	Y	610	CLA	C1A-CHA	2.15	1.52	1.43
28	c	509	CLA	C1A-CHA	2.15	1.52	1.43
28	B	607	CLA	C1A-CHA	2.15	1.52	1.43
28	b	610	CLA	C1A-CHA	2.15	1.52	1.43
28	C	508	CLA	C3B-C2B	-2.15	1.37	1.40
41	d	405	PL9	C6-C1	-2.15	1.44	1.48
28	d	402	CLA	C3B-C2B	-2.15	1.37	1.40
28	c	506	CLA	C1A-CHA	2.15	1.52	1.43
28	N	602	CLA	C3B-C2B	-2.15	1.37	1.40
28	A	410	CLA	C1A-CHA	2.15	1.52	1.43
28	b	615	CLA	C1A-CHA	2.14	1.52	1.43
28	C	506	CLA	C1A-CHA	2.14	1.52	1.43
28	C	511	CLA	C3B-C2B	-2.14	1.37	1.40
28	G	610	CLA	C3B-C2B	-2.14	1.37	1.40
28	C	509	CLA	C1A-CHA	2.14	1.52	1.43
28	b	604	CLA	C1A-CHA	2.14	1.52	1.43
28	B	603	CLA	C1C-C2C	2.14	1.48	1.44
28	d	403	CLA	C1C-C2C	2.14	1.48	1.44
28	G	614	CLA	C1C-C2C	2.14	1.48	1.44
36	S	626	3PH	O21-C21	2.14	1.40	1.34
28	S	613	CLA	C1C-C2C	2.14	1.48	1.44
28	b	603	CLA	C1A-CHA	2.14	1.52	1.43
36	T	101	3PH	O31-C3	-2.14	1.40	1.45
28	c	505	CLA	C1C-C2C	2.14	1.48	1.44
28	c	511	CLA	C1C-C2C	2.14	1.48	1.44
28	b	617	CLA	C1A-CHA	2.14	1.52	1.43
29	a	408	PHO	CMC-C2C	-2.14	1.46	1.51
28	Y	602	CLA	C1C-C2C	2.14	1.48	1.44
37	C	524	DGA	OG2-CG2	-2.13	1.41	1.46
36	b	624	3PH	O21-C21	2.13	1.40	1.34
28	C	501	CLA	C1B-NB	2.13	1.37	1.35
46	G	608	CHL	C3B-C2B	-2.13	1.37	1.40
28	C	502	CLA	C1A-CHA	2.13	1.52	1.43
42	F	101	HEM	FE-ND	2.13	2.07	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	409	PHO	CMC-C2C	-2.13	1.46	1.51
46	S	601	CHL	C3B-C2B	-2.13	1.37	1.40
28	C	507	CLA	C1A-CHA	2.13	1.51	1.43
28	B	611	CLA	C1A-CHA	2.13	1.51	1.43
28	A	410	CLA	C1C-C2C	2.13	1.48	1.44
28	S	610	CLA	C1C-C2C	2.13	1.48	1.44
28	S	609	CLA	C1C-C2C	2.13	1.48	1.44
29	a	409	PHO	CMD-C2D	-2.13	1.46	1.51
28	C	511	CLA	C1A-CHA	2.13	1.51	1.43
28	G	602	CLA	C1A-CHA	2.13	1.51	1.43
28	a	410	CLA	C1A-CHA	2.12	1.51	1.43
28	N	602	CLA	C1C-C2C	2.12	1.48	1.44
28	B	604	CLA	C1A-CHA	2.12	1.51	1.43
28	G	610	CLA	C1A-CHA	2.12	1.51	1.43
28	S	610	CLA	C1A-CHA	2.12	1.51	1.43
28	Y	604	CLA	C1A-CHA	2.12	1.51	1.43
28	N	612	CLA	C1C-C2C	2.12	1.48	1.44
28	B	610	CLA	C1A-CHA	2.11	1.51	1.43
28	Y	612	CLA	C1C-C2C	2.11	1.48	1.44
28	c	507	CLA	C1A-CHA	2.11	1.51	1.43
28	b	613	CLA	C1A-CHA	2.11	1.51	1.43
28	G	604	CLA	C1C-C2C	2.11	1.48	1.44
28	N	602	CLA	C1B-NB	2.11	1.37	1.35
28	C	501	CLA	C1A-CHA	2.11	1.51	1.43
28	c	512	CLA	C1C-C2C	2.11	1.48	1.44
36	B	624	3PH	O31-C3	-2.11	1.40	1.45
28	B	615	CLA	C1A-CHA	2.11	1.51	1.43
46	G	601	CHL	C3B-C2B	-2.11	1.37	1.40
28	b	614	CLA	C1C-C2C	2.11	1.48	1.44
28	G	604	CLA	C1A-CHA	2.11	1.51	1.43
28	B	604	CLA	C1C-C2C	2.11	1.48	1.44
28	B	606	CLA	C1A-CHA	2.11	1.51	1.43
28	B	605	CLA	C3B-C2B	-2.11	1.37	1.40
41	D	405	PL9	C53-C6	-2.10	1.46	1.50
28	Y	603	CLA	C1A-CHA	2.10	1.51	1.43
29	a	409	PHO	CMC-C2C	-2.10	1.46	1.51
46	S	607	CHL	C3B-C2B	-2.10	1.37	1.40
28	Y	611	CLA	C1C-C2C	2.10	1.48	1.44
28	S	603	CLA	C1C-C2C	2.10	1.48	1.44
28	C	510	CLA	C3D-C4D	-2.10	1.39	1.44
28	c	510	CLA	C1A-CHA	2.10	1.51	1.43
28	D	403	CLA	C1A-CHA	2.10	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	605	CLA	C1C-C2C	2.10	1.48	1.44
36	b	624	3PH	O31-C3	-2.10	1.40	1.45
28	S	605	CLA	MG-NC	2.10	2.11	2.06
29	A	408	PHO	CMC-C2C	-2.10	1.46	1.51
28	S	614	CLA	C1A-CHA	2.10	1.51	1.43
42	F	101	HEM	CMB-C2B	2.09	1.55	1.50
28	c	503	CLA	C1A-CHA	2.09	1.51	1.43
37	j	101	DGA	OG2-CG2	-2.09	1.41	1.46
28	G	612	CLA	C1C-C2C	2.09	1.48	1.44
28	B	615	CLA	C1C-C2C	2.09	1.48	1.44
28	D	402	CLA	C1C-C2C	2.09	1.48	1.44
28	b	608	CLA	C1C-C2C	2.09	1.48	1.44
28	S	602	CLA	C1C-C2C	2.09	1.48	1.44
28	b	611	CLA	C1A-CHA	2.09	1.51	1.43
28	C	511	CLA	C1C-C2C	2.09	1.48	1.44
28	b	616	CLA	C1C-C2C	2.09	1.48	1.44
28	G	614	CLA	C3B-C2B	-2.09	1.37	1.40
28	a	405	CLA	C1A-CHA	2.09	1.51	1.43
36	t	101	3PH	O31-C3	-2.09	1.40	1.45
28	Y	610	CLA	C3B-C2B	-2.09	1.37	1.40
28	S	602	CLA	C1A-CHA	2.09	1.51	1.43
28	c	505	CLA	C3B-C2B	-2.09	1.37	1.40
28	Y	610	CLA	C1C-C2C	2.09	1.48	1.44
28	Y	603	CLA	C1C-C2C	2.08	1.48	1.44
42	f	101	HEM	CMB-C2B	2.08	1.55	1.50
37	c	524	DGA	OG2-CG2	-2.08	1.41	1.46
28	b	603	CLA	C1B-NB	2.08	1.37	1.35
28	B	613	CLA	C1A-CHA	2.08	1.51	1.43
28	D	403	CLA	C1B-NB	2.08	1.37	1.35
29	A	408	PHO	CMD-C2D	-2.08	1.46	1.51
28	S	617	CLA	C1C-C2C	2.08	1.48	1.44
29	A	409	PHO	CMD-C2D	-2.08	1.46	1.51
28	B	616	CLA	C1C-C2C	2.08	1.48	1.44
28	a	407	CLA	C3D-C4D	-2.08	1.39	1.44
28	C	507	CLA	C3D-C4D	-2.08	1.39	1.44
36	S	626	3PH	O31-C3	-2.07	1.40	1.45
28	b	607	CLA	C1C-C2C	2.07	1.48	1.44
36	T	101	3PH	O21-C2	-2.07	1.41	1.46
28	Y	602	CLA	C1A-CHA	2.07	1.51	1.43
28	S	605	CLA	C3D-C4D	-2.07	1.39	1.44
28	B	607	CLA	C3B-C2B	-2.07	1.37	1.40
28	b	612	CLA	C1A-CHA	2.07	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y	604	CLA	C1C-C2C	2.07	1.48	1.44
28	B	603	CLA	C1B-NB	2.07	1.37	1.35
28	S	614	CLA	C1C-C2C	2.06	1.48	1.44
28	Y	614	CLA	C1C-C2C	2.06	1.48	1.44
28	c	508	CLA	C1A-CHA	2.06	1.51	1.43
28	C	505	CLA	C1C-C2C	2.06	1.48	1.44
28	b	602	CLA	C1C-C2C	2.06	1.48	1.44
28	a	406	CLA	C1C-C2C	2.06	1.48	1.44
28	B	612	CLA	C3B-C2B	-2.06	1.37	1.40
49	G	623	NEX	C2-C3	2.06	1.55	1.52
28	B	612	CLA	C1A-CHA	2.06	1.51	1.43
28	B	609	CLA	C3D-C4D	-2.06	1.39	1.44
28	N	611	CLA	C1C-C2C	2.06	1.48	1.44
41	d	405	PL9	C26-C24	-2.06	1.47	1.51
28	A	405	CLA	C1A-CHA	2.06	1.51	1.43
42	f	101	HEM	FE-NB	2.06	2.07	1.96
28	Y	611	CLA	C3B-C2B	-2.06	1.37	1.40
29	a	408	PHO	CMB-C2B	-2.06	1.46	1.51
29	a	408	PHO	CMD-C2D	-2.06	1.46	1.51
28	S	602	CLA	C3B-C2B	-2.06	1.37	1.40
28	N	603	CLA	C1C-C2C	2.06	1.48	1.44
28	N	613	CLA	MG-NC	2.05	2.11	2.06
32	h	102	LMG	C22-C21	-2.05	1.33	1.49
28	N	604	CLA	C1C-C2C	2.05	1.48	1.44
37	J	101	DGA	OG2-CG2	-2.05	1.41	1.46
28	C	508	CLA	C1A-CHA	2.05	1.51	1.43
28	Y	608	CLA	C1B-NB	2.05	1.37	1.35
46	S	608	CHL	C3B-C2B	-2.05	1.37	1.40
28	c	507	CLA	C3D-C4D	-2.05	1.39	1.44
28	S	603	CLA	MG-NC	2.05	2.11	2.06
28	b	607	CLA	C3D-C4D	-2.04	1.39	1.44
28	S	611	CLA	MG-NC	2.04	2.11	2.06
28	G	611	CLA	MG-NC	2.04	2.11	2.06
28	N	611	CLA	C1B-NB	2.04	1.37	1.35
28	A	407	CLA	C1C-C2C	2.04	1.48	1.44
32	A	413	LMG	C43-C42	-2.04	1.33	1.49
28	C	507	CLA	C1C-C2C	2.04	1.48	1.44
28	S	611	CLA	C1C-C2C	2.03	1.48	1.44
32	h	102	LMG	O1-C1	2.03	1.43	1.40
51	Y	627	PTY	O4-C1	-2.03	1.40	1.45
28	b	602	CLA	MG-NC	2.03	2.11	2.06
28	d	402	CLA	C3D-C4D	-2.03	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	503	CLA	C3B-C2B	-2.02	1.37	1.40
28	B	607	CLA	C3D-C4D	-2.02	1.39	1.44
28	N	612	CLA	MG-NC	2.02	2.11	2.06
28	N	604	CLA	C3D-C4D	-2.02	1.39	1.44
28	B	604	CLA	C3D-C4D	-2.02	1.39	1.44
28	S	617	CLA	C1B-NB	2.02	1.37	1.35
28	c	501	CLA	C1B-NB	2.02	1.37	1.35
28	D	402	CLA	C3D-C4D	-2.02	1.39	1.44
35	C	518	DGD	CGB-CFB	-2.02	1.33	1.49
49	N	623	NEX	C1-C6	-2.02	1.51	1.54
28	G	614	CLA	C1B-NB	2.02	1.37	1.35
28	b	608	CLA	C3B-C2B	-2.02	1.37	1.40
28	B	608	CLA	C3D-C4D	-2.02	1.39	1.44
29	A	409	PHO	CMB-C2B	-2.02	1.46	1.51
28	B	609	CLA	C1C-C2C	2.02	1.48	1.44
28	b	605	CLA	C1C-C2C	2.02	1.48	1.44
28	C	505	CLA	C3D-C4D	-2.02	1.39	1.44
28	A	405	CLA	C3D-C4D	-2.02	1.39	1.44
29	A	408	PHO	CMB-C2B	-2.02	1.46	1.51
46	N	601	CHL	C3B-C2B	-2.01	1.37	1.40
28	Y	602	CLA	C3B-C2B	-2.01	1.37	1.40
35	C	519	DGD	CGB-CFB	-2.01	1.33	1.49
28	B	602	CLA	MG-NC	2.01	2.11	2.06
28	B	613	CLA	C3D-C4D	-2.01	1.39	1.44
35	c	520	DGD	CDA-CCA	-2.01	1.33	1.49
35	c	519	DGD	CGB-CFB	-2.01	1.33	1.49
28	C	503	CLA	MG-NC	2.01	2.11	2.06
28	G	604	CLA	C1B-NB	2.01	1.37	1.35
28	G	604	CLA	C3D-C4D	-2.01	1.39	1.44
35	C	520	DGD	CDA-CCA	-2.01	1.33	1.49
28	b	605	CLA	MG-NC	2.01	2.11	2.06
28	N	614	CLA	C1B-NB	2.01	1.37	1.35
28	b	604	CLA	C1C-C2C	2.01	1.48	1.44
28	C	507	CLA	C3B-C2B	-2.01	1.37	1.40
28	S	604	CLA	CHD-C1D	2.01	1.42	1.38
28	C	509	CLA	C3D-C4D	-2.01	1.39	1.44
28	B	613	CLA	C1C-C2C	2.01	1.48	1.44
28	a	405	CLA	C1C-C2C	2.01	1.48	1.44
28	N	614	CLA	MG-NC	2.01	2.11	2.06
28	G	611	CLA	CHD-C1D	2.01	1.42	1.38
35	C	520	DGD	CGB-CFB	-2.01	1.33	1.49
28	Y	608	CLA	MG-NC	2.01	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	510	CLA	C1C-C2C	2.01	1.48	1.44
32	A	413	LMG	C22-C21	-2.01	1.33	1.49
28	Y	611	CLA	MG-NC	2.01	2.11	2.06
32	H	102	LMG	C43-C42	-2.01	1.33	1.49
32	C	521	LMG	C43-C42	-2.00	1.33	1.49
28	N	613	CLA	C1B-NB	2.00	1.37	1.35
32	H	102	LMG	C22-C21	-2.00	1.33	1.49
32	a	413	LMG	C22-C21	-2.00	1.33	1.49
32	h	102	LMG	C43-C42	-2.00	1.33	1.49
32	B	622	LMG	C25-C24	-2.00	1.33	1.49
51	Y	626	PTY	O4-C1	-2.00	1.40	1.45
35	c	520	DGD	CGB-CFB	-2.00	1.33	1.49
28	B	615	CLA	C3D-C4D	-2.00	1.39	1.44
28	Y	612	CLA	MG-NC	2.00	2.11	2.06
28	B	616	CLA	C1B-NB	2.00	1.37	1.35
28	B	607	CLA	C1C-C2C	2.00	1.48	1.44
32	C	521	LMG	C25-C24	-2.00	1.33	1.49

All (2768) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	l	101	LHG	O7-C7-C8	23.08	161.24	111.50
38	L	101	LHG	O7-C7-C8	22.88	160.81	111.50
36	S	626	3PH	O21-C21-C22	22.37	159.71	111.50
30	b	618	BCR	C10-C11-C12	18.18	179.96	123.22
36	S	626	3PH	O21-C21-O22	-18.16	79.82	123.70
38	L	101	LHG	O7-C7-O9	-18.13	79.88	123.70
38	l	101	LHG	O7-C7-O9	-17.93	80.36	123.70
30	B	618	BCR	C10-C11-C12	17.88	179.02	123.22
30	C	515	BCR	C10-C11-C12	17.76	178.66	123.22
30	c	514	BCR	C10-C11-C12	17.70	178.47	123.22
30	C	517	BCR	C10-C11-C12	17.58	178.09	123.22
30	c	516	BCR	C10-C11-C12	17.53	177.91	123.22
30	C	516	BCR	C10-C11-C12	17.52	177.88	123.22
30	A	411	BCR	C10-C11-C12	17.52	177.88	123.22
30	C	514	BCR	C10-C11-C12	17.47	177.74	123.22
30	d	404	BCR	C10-C11-C12	17.41	177.54	123.22
30	b	619	BCR	C10-C11-C12	17.40	177.52	123.22
30	c	517	BCR	C10-C11-C12	17.38	177.45	123.22
30	a	411	BCR	C10-C11-C12	17.31	177.22	123.22
30	B	619	BCR	C10-C11-C12	17.27	177.11	123.22
30	c	515	BCR	C10-C11-C12	17.25	177.05	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	404	BCR	C10-C11-C12	17.24	177.01	123.22
48	Y	622	XAT	C37-C21-C36	-16.67	82.78	107.37
30	c	514	BCR	C16-C15-C14	15.35	154.92	123.47
30	c	516	BCR	C16-C15-C14	15.25	154.72	123.47
30	C	514	BCR	C16-C15-C14	15.00	154.20	123.47
30	c	517	BCR	C16-C15-C14	14.40	152.97	123.47
30	b	619	BCR	C16-C15-C14	14.39	152.94	123.47
30	b	618	BCR	C16-C15-C14	14.29	152.75	123.47
30	B	618	BCR	C16-C15-C14	14.23	152.63	123.47
30	C	516	BCR	C11-C10-C9	14.07	147.40	127.31
30	c	515	BCR	C16-C15-C14	14.02	152.19	123.47
30	d	404	BCR	C16-C15-C14	13.92	151.98	123.47
30	C	515	BCR	C16-C15-C14	13.60	151.34	123.47
30	C	517	BCR	C21-C20-C19	13.39	164.99	123.22
30	c	516	BCR	C11-C10-C9	13.21	146.16	127.31
30	b	618	BCR	C11-C10-C9	13.13	146.04	127.31
30	B	618	BCR	C11-C10-C9	13.11	146.03	127.31
30	C	516	BCR	C16-C15-C14	13.03	150.17	123.47
30	c	517	BCR	C21-C20-C19	12.84	163.28	123.22
30	c	517	BCR	C11-C10-C9	12.81	145.60	127.31
30	C	514	BCR	C11-C10-C9	12.80	145.57	127.31
48	Y	622	XAT	C37-C21-C22	-12.76	86.80	108.98
30	D	404	BCR	C21-C20-C19	12.75	163.01	123.22
30	b	619	BCR	C11-C10-C9	12.68	145.40	127.31
30	c	516	BCR	C21-C20-C19	12.59	162.51	123.22
30	B	619	BCR	C16-C15-C14	12.57	149.22	123.47
30	A	411	BCR	C11-C10-C9	12.54	145.21	127.31
30	a	411	BCR	C21-C20-C19	12.52	162.28	123.22
30	a	411	BCR	C11-C10-C9	12.43	145.05	127.31
30	C	516	BCR	C21-C20-C19	12.43	162.01	123.22
30	d	404	BCR	C11-C10-C9	12.39	144.99	127.31
30	D	404	BCR	C16-C15-C14	12.38	148.84	123.47
30	c	514	BCR	C21-C20-C19	12.36	161.78	123.22
30	A	411	BCR	C21-C20-C19	12.35	161.77	123.22
30	a	411	BCR	C16-C15-C14	12.30	148.66	123.47
30	C	517	BCR	C11-C10-C9	12.26	144.81	127.31
30	B	619	BCR	C21-C20-C19	12.18	161.23	123.22
30	c	514	BCR	C11-C10-C9	12.08	144.55	127.31
30	A	411	BCR	C16-C15-C14	12.05	148.16	123.47
30	d	404	BCR	C21-C20-C19	12.04	160.80	123.22
30	B	619	BCR	C11-C10-C9	12.03	144.48	127.31
30	C	517	BCR	C16-C15-C14	11.99	148.03	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	618	BCR	C21-C20-C19	11.91	160.38	123.22
30	b	619	BCR	C21-C20-C19	11.69	159.70	123.22
30	c	515	BCR	C21-C20-C19	11.50	159.11	123.22
30	B	618	BCR	C21-C20-C19	11.26	158.35	123.22
36	S	626	3PH	O22-C21-C22	-11.24	79.90	123.73
30	C	514	BCR	C21-C20-C19	11.20	158.17	123.22
30	D	404	BCR	C11-C10-C9	11.18	143.27	127.31
30	C	515	BCR	C11-C10-C9	11.14	143.20	127.31
30	B	619	BCR	C11-C12-C13	11.03	157.40	126.42
38	L	101	LHG	O9-C7-C8	-10.97	80.95	123.73
38	l	101	LHG	O9-C7-C8	-10.95	81.03	123.73
30	D	404	BCR	C11-C12-C13	10.66	156.36	126.42
30	b	618	BCR	C11-C12-C13	10.65	156.34	126.42
30	a	411	BCR	C11-C12-C13	10.63	156.29	126.42
30	c	515	BCR	C11-C10-C9	10.52	142.33	127.31
30	C	515	BCR	C11-C12-C13	10.50	155.92	126.42
30	C	517	BCR	C11-C12-C13	10.47	155.83	126.42
30	A	411	BCR	C11-C12-C13	10.44	155.75	126.42
30	d	404	BCR	C11-C12-C13	10.38	155.57	126.42
30	c	517	BCR	C11-C12-C13	10.36	155.52	126.42
30	C	516	BCR	C11-C12-C13	10.18	155.02	126.42
30	c	515	BCR	C11-C12-C13	10.14	154.91	126.42
28	a	407	CLA	C4A-NA-C1A	10.07	111.23	106.71
30	C	515	BCR	C21-C20-C19	10.06	154.62	123.22
30	B	618	BCR	C11-C12-C13	10.04	154.62	126.42
30	b	619	BCR	C11-C12-C13	9.94	154.35	126.42
28	b	606	CLA	C4A-NA-C1A	9.93	111.17	106.71
30	c	514	BCR	C11-C12-C13	9.93	154.31	126.42
28	B	605	CLA	C4A-NA-C1A	9.79	111.11	106.71
30	C	514	BCR	C11-C12-C13	9.76	153.82	126.42
28	c	505	CLA	C4A-NA-C1A	9.69	111.06	106.71
28	c	512	CLA	C4A-NA-C1A	9.65	111.05	106.71
28	c	513	CLA	C4A-NA-C1A	9.61	111.03	106.71
28	A	406	CLA	C4A-NA-C1A	9.58	111.02	106.71
28	C	513	CLA	C4A-NA-C1A	9.57	111.01	106.71
28	b	610	CLA	C4A-NA-C1A	9.56	111.01	106.71
28	N	610	CLA	C4A-NA-C1A	9.56	111.00	106.71
28	a	405	CLA	C4A-NA-C1A	9.53	110.99	106.71
28	C	504	CLA	C4A-NA-C1A	9.52	110.99	106.71
28	S	603	CLA	C4A-NA-C1A	9.47	110.97	106.71
28	G	603	CLA	C4A-NA-C1A	9.39	110.93	106.71
28	B	606	CLA	C4A-NA-C1A	9.39	110.93	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	609	CLA	C4A-NA-C1A	9.37	110.92	106.71
28	C	512	CLA	C4A-NA-C1A	9.34	110.90	106.71
28	c	504	CLA	C4A-NA-C1A	9.32	110.89	106.71
28	c	510	CLA	C4A-NA-C1A	9.32	110.89	106.71
28	S	611	CLA	C4A-NA-C1A	9.31	110.89	106.71
28	Y	612	CLA	C4A-NA-C1A	9.30	110.89	106.71
28	Y	603	CLA	C4A-NA-C1A	9.29	110.88	106.71
28	N	613	CLA	C4A-NA-C1A	9.28	110.88	106.71
28	C	509	CLA	C4A-NA-C1A	9.27	110.88	106.71
30	c	516	BCR	C11-C12-C13	9.27	152.45	126.42
28	S	617	CLA	C4A-NA-C1A	9.26	110.87	106.71
28	C	502	CLA	C4A-NA-C1A	9.24	110.86	106.71
28	B	602	CLA	C4A-NA-C1A	9.24	110.86	106.71
30	C	515	BCR	C20-C19-C18	9.23	152.35	126.42
28	N	614	CLA	C4A-NA-C1A	9.23	110.86	106.71
28	b	608	CLA	C4A-NA-C1A	9.23	110.86	106.71
28	B	608	CLA	C4A-NA-C1A	9.22	110.85	106.71
28	C	510	CLA	C4A-NA-C1A	9.22	110.85	106.71
28	N	603	CLA	C4A-NA-C1A	9.22	110.85	106.71
28	B	613	CLA	C4A-NA-C1A	9.21	110.84	106.71
28	B	614	CLA	C4A-NA-C1A	9.19	110.84	106.71
28	B	617	CLA	C4A-NA-C1A	9.19	110.84	106.71
28	c	509	CLA	C4A-NA-C1A	9.17	110.83	106.71
28	b	614	CLA	C4A-NA-C1A	9.17	110.83	106.71
28	S	613	CLA	C4A-NA-C1A	9.17	110.83	106.71
28	c	511	CLA	C4A-NA-C1A	9.12	110.81	106.71
28	C	511	CLA	C4A-NA-C1A	9.09	110.79	106.71
28	S	604	CLA	C4A-NA-C1A	9.08	110.79	106.71
28	b	605	CLA	C4A-NA-C1A	9.07	110.78	106.71
28	Y	613	CLA	C4A-NA-C1A	9.06	110.78	106.71
28	N	604	CLA	C4A-NA-C1A	9.05	110.78	106.71
28	c	506	CLA	C4A-NA-C1A	9.04	110.77	106.71
28	A	407	CLA	C4A-NA-C1A	9.04	110.77	106.71
28	S	609	CLA	C4A-NA-C1A	9.03	110.76	106.71
28	B	615	CLA	C4A-NA-C1A	9.02	110.76	106.71
28	b	617	CLA	C4A-NA-C1A	9.01	110.76	106.71
28	c	502	CLA	C4A-NA-C1A	9.00	110.75	106.71
28	B	603	CLA	C4A-NA-C1A	8.99	110.75	106.71
28	b	612	CLA	C4A-NA-C1A	8.97	110.74	106.71
28	B	612	CLA	C4A-NA-C1A	8.93	110.72	106.71
28	G	613	CLA	C4A-NA-C1A	8.91	110.71	106.71
28	G	614	CLA	C4A-NA-C1A	8.90	110.71	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	610	CLA	C4A-NA-C1A	8.89	110.70	106.71
28	N	611	CLA	C4A-NA-C1A	8.88	110.70	106.71
28	b	602	CLA	C4A-NA-C1A	8.87	110.69	106.71
28	b	615	CLA	C4A-NA-C1A	8.83	110.68	106.71
28	A	410	CLA	C4A-NA-C1A	8.83	110.67	106.71
28	b	603	CLA	C4A-NA-C1A	8.83	110.67	106.71
28	Y	610	CLA	C4A-NA-C1A	8.82	110.67	106.71
28	C	506	CLA	C4A-NA-C1A	8.82	110.67	106.71
28	G	604	CLA	C4A-NA-C1A	8.81	110.67	106.71
28	S	612	CLA	C4A-NA-C1A	8.81	110.67	106.71
28	b	616	CLA	C4A-NA-C1A	8.81	110.67	106.71
28	Y	608	CLA	C4A-NA-C1A	8.81	110.67	106.71
28	d	403	CLA	C4A-NA-C1A	8.79	110.66	106.71
28	Y	611	CLA	C4A-NA-C1A	8.78	110.65	106.71
28	c	508	CLA	C4A-NA-C1A	8.78	110.65	106.71
28	G	610	CLA	C4A-NA-C1A	8.76	110.65	106.71
28	B	607	CLA	C4A-NA-C1A	8.74	110.64	106.71
28	S	605	CLA	C4A-NA-C1A	8.74	110.64	106.71
28	C	505	CLA	C4A-NA-C1A	8.73	110.63	106.71
28	Y	614	CLA	C4A-NA-C1A	8.73	110.63	106.71
28	Y	604	CLA	C4A-NA-C1A	8.71	110.62	106.71
28	c	507	CLA	C4A-NA-C1A	8.70	110.62	106.71
28	D	403	CLA	C4A-NA-C1A	8.68	110.61	106.71
28	C	507	CLA	C4A-NA-C1A	8.67	110.60	106.71
28	C	501	CLA	C4A-NA-C1A	8.66	110.60	106.71
28	b	613	CLA	C4A-NA-C1A	8.65	110.59	106.71
28	G	602	CLA	C4A-NA-C1A	8.63	110.59	106.71
28	A	405	CLA	C4A-NA-C1A	8.62	110.58	106.71
28	C	503	CLA	C4A-NA-C1A	8.62	110.58	106.71
28	G	612	CLA	C4A-NA-C1A	8.62	110.58	106.71
28	b	607	CLA	C4A-NA-C1A	8.61	110.58	106.71
28	Y	602	CLA	C4A-NA-C1A	8.60	110.57	106.71
28	G	611	CLA	C4A-NA-C1A	8.60	110.57	106.71
28	c	501	CLA	C4A-NA-C1A	8.59	110.57	106.71
30	B	618	BCR	C20-C19-C18	8.57	150.50	126.42
28	B	616	CLA	C4A-NA-C1A	8.55	110.55	106.71
28	B	609	CLA	C4A-NA-C1A	8.55	110.55	106.71
28	b	611	CLA	C4A-NA-C1A	8.55	110.55	106.71
30	C	514	BCR	C20-C19-C18	8.55	150.44	126.42
28	N	602	CLA	C4A-NA-C1A	8.55	110.55	106.71
28	a	410	CLA	C4A-NA-C1A	8.55	110.55	106.71
28	S	602	CLA	C4A-NA-C1A	8.54	110.55	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	604	CLA	C4A-NA-C1A	8.53	110.54	106.71
28	N	612	CLA	C4A-NA-C1A	8.49	110.53	106.71
28	S	610	CLA	C4A-NA-C1A	8.48	110.52	106.71
28	D	402	CLA	C4A-NA-C1A	8.47	110.52	106.71
28	c	503	CLA	C4A-NA-C1A	8.47	110.51	106.71
28	B	604	CLA	C4A-NA-C1A	8.35	110.46	106.71
30	b	618	BCR	C20-C19-C18	8.35	149.88	126.42
28	a	406	CLA	C4A-NA-C1A	8.34	110.45	106.71
28	B	611	CLA	C4A-NA-C1A	8.33	110.45	106.71
30	c	515	BCR	C20-C19-C18	8.32	149.79	126.42
30	b	619	BCR	C20-C19-C18	8.32	149.78	126.42
28	S	614	CLA	C4A-NA-C1A	8.31	110.44	106.71
43	H	101	RRX	C38-C26-C25	-8.19	115.33	124.53
30	d	404	BCR	C20-C19-C18	8.05	149.02	126.42
28	C	508	CLA	C4A-NA-C1A	8.03	110.31	106.71
39	C	527	LMK	O2-C4-O3	-7.94	106.06	124.09
30	c	514	BCR	C20-C19-C18	7.78	148.27	126.42
28	d	402	CLA	C4A-NA-C1A	7.77	110.20	106.71
30	C	516	BCR	C20-C19-C18	7.66	147.93	126.42
30	B	619	BCR	C20-C19-C18	7.61	147.78	126.42
43	h	101	RRX	C38-C26-C25	-7.36	116.27	124.53
30	c	517	BCR	C20-C19-C18	7.34	147.04	126.42
48	Y	622	XAT	C36-C21-C22	7.22	121.53	108.98
30	a	411	BCR	C20-C19-C18	7.21	146.68	126.42
30	c	516	BCR	C20-C19-C18	7.20	146.63	126.42
30	A	411	BCR	C20-C19-C18	7.14	146.46	126.42
48	Y	622	XAT	C37-C21-C26	-7.09	90.91	110.05
30	D	404	BCR	C20-C19-C18	6.95	145.93	126.42
37	C	524	DGA	CDB-CCB-CBB	-6.83	79.75	114.42
37	b	625	DGA	CDB-CCB-CBB	-6.82	79.81	114.42
37	B	625	DGA	CDB-CCB-CBB	-6.61	80.85	114.42
30	C	517	BCR	C20-C19-C18	6.60	144.94	126.42
43	H	101	RRX	C15-C14-C13	-6.54	117.97	127.31
28	S	603	CLA	O2D-CGD-CBD	6.52	122.86	111.27
28	S	602	CLA	O2D-CGD-CBD	6.50	122.82	111.27
37	c	524	DGA	CDB-CCB-CBB	-6.49	81.48	114.42
28	B	606	CLA	O2A-C1-C2	6.39	125.43	108.64
39	c	527	LMK	O2-C4-O3	-6.35	109.67	124.09
28	a	407	CLA	CMD-C2D-C1D	6.29	135.80	124.71
28	B	609	CLA	O2D-CGD-CBD	6.21	122.31	111.27
28	b	606	CLA	CMD-C2D-C1D	6.15	135.56	124.71
28	b	612	CLA	O2A-C1-C2	6.08	124.62	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	604	CLA	O2A-C1-C2	6.04	124.52	108.64
28	B	606	CLA	CMD-C2D-C1D	6.04	135.35	124.71
28	b	615	CLA	CMD-C2D-C1D	5.99	135.27	124.71
28	d	402	CLA	O2A-C1-C2	5.99	124.37	108.64
28	c	505	CLA	O2A-C1-C2	5.95	124.28	108.64
28	B	608	CLA	CMD-C2D-C1D	5.91	135.12	124.71
28	B	615	CLA	CMD-C2D-C1D	5.87	135.06	124.71
43	H	101	RRX	C11-C10-C9	-5.86	118.94	127.31
28	c	505	CLA	O2D-CGD-CBD	5.86	121.69	111.27
28	C	507	CLA	O2A-C1-C2	5.85	124.02	108.64
28	C	510	CLA	CMD-C2D-C1D	5.84	135.01	124.71
28	B	605	CLA	O2D-CGD-CBD	5.84	121.64	111.27
43	H	101	RRX	C24-C25-C26	-5.77	107.48	121.46
28	a	406	CLA	CMD-C2D-C1D	5.77	134.88	124.71
28	A	405	CLA	CMD-C2D-C1D	5.76	134.86	124.71
28	G	614	CLA	CMD-C2D-C1D	5.75	134.85	124.71
28	C	511	CLA	CMD-C2D-C1D	5.75	134.84	124.71
28	S	602	CLA	O2A-C1-C2	5.74	123.72	108.64
28	G	604	CLA	O2D-CGD-CBD	5.72	121.43	111.27
48	N	622	XAT	C31-C30-C29	-5.71	119.16	127.31
28	G	614	CLA	O2A-C1-C2	5.68	122.25	108.97
28	a	405	CLA	CMD-C2D-C1D	5.68	134.72	124.71
28	S	614	CLA	CMD-C2D-C1D	5.68	134.72	124.71
28	a	407	CLA	O2D-CGD-CBD	5.67	121.35	111.27
28	C	501	CLA	CMD-C2D-C1D	5.66	134.69	124.71
49	G	623	NEX	C2-C1-C6	5.66	114.71	109.21
28	N	604	CLA	O2D-CGD-CBD	5.65	121.31	111.27
28	C	509	CLA	CMD-C2D-C1D	5.65	134.67	124.71
47	G	621	LUT	C21-C26-C25	5.65	121.54	111.42
28	S	613	CLA	CMD-C2D-C1D	5.64	134.66	124.71
28	N	614	CLA	O2A-C1-C2	5.64	122.15	108.97
34	b	620	C7Z	C38-C25-C26	-5.64	118.20	124.53
28	c	509	CLA	CMD-C2D-C1D	5.63	134.64	124.71
28	N	610	CLA	CMD-C2D-C1D	5.63	134.63	124.71
28	B	614	CLA	CMD-C2D-C1D	5.63	134.63	124.71
28	c	510	CLA	CMD-C2D-C1D	5.61	134.59	124.71
28	Y	613	CLA	CMD-C2D-C1D	5.60	134.58	124.71
28	N	604	CLA	CMD-C2D-C1D	5.58	134.55	124.71
28	c	513	CLA	CMD-C2D-C1D	5.58	134.55	124.71
28	G	604	CLA	CMD-C2D-C1D	5.57	134.53	124.71
28	c	502	CLA	CMD-C2D-C1D	5.57	134.53	124.71
28	C	504	CLA	O2A-C1-C2	5.57	123.27	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	501	CLA	CMD-C2D-C1D	5.56	134.51	124.71
28	B	617	CLA	O2D-CGD-CBD	5.56	121.14	111.27
28	S	611	CLA	O2D-CGD-CBD	5.56	121.14	111.27
28	b	616	CLA	CMD-C2D-C1D	5.56	134.50	124.71
28	N	611	CLA	CMD-C2D-C1D	5.55	134.50	124.71
28	b	609	CLA	O2D-CGD-CBD	5.55	121.12	111.27
28	N	602	CLA	O2D-CGD-CBD	5.54	121.12	111.27
47	N	621	LUT	C21-C26-C25	5.54	121.34	111.42
28	B	603	CLA	O2A-C1-C2	5.54	123.19	108.64
47	Y	621	LUT	C21-C26-C25	5.53	121.33	111.42
28	C	503	CLA	CMD-C2D-C1D	5.53	134.46	124.71
28	B	603	CLA	CMD-C2D-C1D	5.52	134.44	124.71
28	D	403	CLA	CMD-C2D-C1D	5.52	134.44	124.71
28	B	605	CLA	CMD-C2D-C1D	5.51	134.42	124.71
28	B	607	CLA	CMD-C2D-C1D	5.51	134.42	124.71
28	G	613	CLA	O2A-C1-C2	5.51	123.11	108.64
28	d	403	CLA	CMD-C2D-C1D	5.51	134.42	124.71
28	Y	602	CLA	O2D-CGD-CBD	5.51	121.06	111.27
28	c	503	CLA	CMD-C2D-C1D	5.50	134.41	124.71
28	b	607	CLA	CMD-C2D-C1D	5.50	134.41	124.71
28	b	602	CLA	CMD-C2D-C1D	5.50	134.41	124.71
28	Y	604	CLA	CMD-C2D-C1D	5.50	134.40	124.71
28	S	605	CLA	CMD-C2D-C1D	5.49	134.38	124.71
28	C	501	CLA	O2D-CGD-CBD	5.48	121.01	111.27
28	b	614	CLA	CMD-C2D-C1D	5.48	134.37	124.71
28	N	602	CLA	CMD-C2D-C1D	5.48	134.37	124.71
28	b	603	CLA	CMD-C2D-C1D	5.48	134.37	124.71
28	b	610	CLA	O2A-C1-C2	5.48	123.03	108.64
28	C	502	CLA	O2A-C1-C2	5.48	123.03	108.64
34	b	620	C7Z	C15-C14-C13	-5.48	119.50	127.31
28	c	504	CLA	CMD-C2D-C1D	5.47	134.36	124.71
28	D	403	CLA	O2D-CGD-CBD	5.47	120.99	111.27
28	N	604	CLA	O2A-C1-C2	5.47	123.02	108.64
28	G	612	CLA	CMD-C2D-C1D	5.47	134.35	124.71
28	N	603	CLA	CMD-C2D-C1D	5.47	134.34	124.71
28	c	511	CLA	CMD-C2D-C1D	5.46	134.34	124.71
28	S	604	CLA	CMD-C2D-C1D	5.46	134.34	124.71
28	b	605	CLA	CMD-C2D-C1D	5.46	134.34	124.71
28	b	603	CLA	O2A-C1-C2	5.46	122.99	108.64
47	S	621	LUT	C21-C26-C25	5.46	121.20	111.42
28	b	608	CLA	O2A-C1-C2	5.45	122.97	108.64
28	B	607	CLA	O2D-CGD-CBD	5.45	120.96	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	507	CLA	CMD-C2D-C1D	5.45	134.32	124.71
28	Y	608	CLA	CMD-C2D-C1D	5.45	134.32	124.71
28	b	610	CLA	CMD-C2D-C1D	5.45	134.31	124.71
28	G	603	CLA	CMD-C2D-C1D	5.45	134.31	124.71
28	S	605	CLA	O2A-C1-C2	5.44	122.94	108.64
28	a	407	CLA	O2A-C1-C2	5.44	121.69	108.97
28	B	602	CLA	CMD-C2D-C1D	5.43	134.28	124.71
28	N	614	CLA	CMD-C2D-C1D	5.42	134.27	124.71
48	N	622	XAT	C15-C14-C13	-5.42	119.57	127.31
47	G	620	LUT	C21-C26-C25	5.42	121.12	111.42
28	S	610	CLA	CMD-C2D-C1D	5.41	134.26	124.71
28	S	604	CLA	O2D-CGD-CBD	5.41	120.89	111.27
28	B	609	CLA	CMD-C2D-C1D	5.41	134.25	124.71
28	C	513	CLA	O2A-C1-C2	5.41	122.85	108.64
28	b	604	CLA	CMD-C2D-C1D	5.41	134.24	124.71
28	Y	610	CLA	CMD-C2D-C1D	5.41	134.24	124.71
28	b	608	CLA	CMD-C2D-C1D	5.40	134.23	124.71
28	C	504	CLA	CMD-C2D-C1D	5.40	134.22	124.71
28	B	604	CLA	CMD-C2D-C1D	5.40	134.22	124.71
28	b	611	CLA	CMD-C2D-C1D	5.40	134.22	124.71
28	c	504	CLA	O2A-C1-C2	5.40	122.81	108.64
28	N	612	CLA	CMD-C2D-C1D	5.39	134.22	124.71
28	A	406	CLA	CMD-C2D-C1D	5.39	134.21	124.71
28	G	603	CLA	O2A-C1-C2	5.39	122.79	108.64
47	Y	620	LUT	C21-C26-C25	5.39	121.07	111.42
28	G	612	CLA	O2D-CGD-CBD	5.38	120.83	111.27
28	C	506	CLA	CMD-C2D-C1D	5.38	134.19	124.71
48	G	622	XAT	C15-C14-C13	-5.37	119.65	127.31
28	S	602	CLA	CMD-C2D-C1D	5.37	134.17	124.71
28	b	613	CLA	O2D-CGD-CBD	5.37	120.80	111.27
28	Y	603	CLA	CMD-C2D-C1D	5.37	134.17	124.71
28	N	613	CLA	O2A-C1-C2	5.36	122.73	108.64
40	d	401	BCT	O2-C-O1	5.36	133.45	119.55
28	G	610	CLA	CMD-C2D-C1D	5.36	134.15	124.71
28	C	509	CLA	O2D-CGD-CBD	5.35	120.78	111.27
28	b	617	CLA	O2D-CGD-CBD	5.35	120.78	111.27
28	A	410	CLA	O2D-CGD-CBD	5.34	120.76	111.27
28	G	610	CLA	O2A-C1-C2	5.34	122.66	108.64
28	B	613	CLA	O2D-CGD-CBD	5.33	120.75	111.27
28	B	612	CLA	O2D-CGD-CBD	5.33	120.74	111.27
28	d	403	CLA	O2D-CGD-CBD	5.33	120.74	111.27
28	Y	603	CLA	O2D-CGD-CBD	5.33	120.73	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	407	CLA	O2D-CGD-CBD	5.32	120.73	111.27
34	B	620	C7Z	C15-C14-C13	-5.32	119.72	127.31
28	c	511	CLA	O2A-C1-C2	5.32	122.62	108.64
28	B	613	CLA	CMD-C2D-C1D	5.32	134.09	124.71
28	G	611	CLA	O2D-CGD-CBD	5.32	120.72	111.27
28	c	507	CLA	CMD-C2D-C1D	5.32	134.08	124.71
40	D	401	BCT	O2-C-O1	5.31	133.32	119.55
28	B	611	CLA	CMD-C2D-C1D	5.31	134.07	124.71
28	c	507	CLA	O2A-C1-C2	5.31	122.58	108.64
28	Y	614	CLA	CMD-C2D-C1D	5.30	134.06	124.71
28	C	502	CLA	CMD-C2D-C1D	5.30	134.06	124.71
28	D	402	CLA	O2A-C1-C2	5.30	122.56	108.64
28	G	602	CLA	O2D-CGD-CBD	5.29	120.67	111.27
28	c	506	CLA	CMD-C2D-C1D	5.29	134.03	124.71
28	Y	611	CLA	CMD-C2D-C1D	5.27	134.01	124.71
28	A	410	CLA	CMD-C2D-C1D	5.27	134.00	124.71
28	b	606	CLA	O2A-C1-C2	5.27	122.48	108.64
28	N	613	CLA	CMD-C2D-C1D	5.27	134.00	124.71
48	Y	622	XAT	C31-C30-C29	-5.27	119.79	127.31
28	G	611	CLA	CMD-C2D-C1D	5.26	133.99	124.71
28	B	605	CLA	O2A-C1-C2	5.26	122.47	108.64
28	Y	610	CLA	O2A-C1-C2	5.26	122.45	108.64
34	B	620	C7Z	C11-C10-C9	-5.26	119.81	127.31
28	Y	602	CLA	CMD-C2D-C1D	5.26	133.98	124.71
35	B	623	DGD	O2G-C1B-C2B	5.26	122.83	111.50
28	C	505	CLA	O2A-C1-C2	5.25	122.44	108.64
28	C	513	CLA	O2D-CGD-CBD	5.25	120.59	111.27
28	B	607	CLA	O2A-C1-C2	5.25	122.42	108.64
28	G	614	CLA	O2D-CGD-CBD	5.24	120.57	111.27
28	A	407	CLA	CMD-C2D-C1D	5.24	133.94	124.71
28	c	508	CLA	CMD-C2D-C1D	5.24	133.94	124.71
28	B	611	CLA	O2D-CGD-CBD	5.23	120.56	111.27
41	d	405	PL9	C7-C3-C4	5.23	121.13	116.88
28	B	616	CLA	CMD-C2D-C1D	5.23	133.93	124.71
28	C	503	CLA	O2D-CGD-CBD	5.22	120.55	111.27
28	C	506	CLA	O2D-CGD-CBD	5.22	120.54	111.27
28	S	609	CLA	CMD-C2D-C1D	5.22	133.91	124.71
28	a	410	CLA	CMD-C2D-C1D	5.22	133.91	124.71
28	S	605	CLA	O2D-CGD-CBD	5.22	120.54	111.27
28	N	603	CLA	O2D-CGD-CBD	5.21	120.53	111.27
28	C	512	CLA	O2D-CGD-CBD	5.21	120.52	111.27
47	G	621	LUT	C21-C26-C27	5.20	119.28	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	602	CLA	O2A-C1-C2	5.20	122.31	108.64
28	S	609	CLA	O2D-CGD-CBD	5.20	120.51	111.27
28	B	617	CLA	O2A-C1-C2	5.20	122.30	108.64
28	Y	604	CLA	O2D-CGD-CBD	5.20	120.50	111.27
28	S	617	CLA	CMD-C2D-C1D	5.20	133.87	124.71
28	c	512	CLA	O2D-CGD-CBD	5.19	120.49	111.27
28	B	602	CLA	O2D-CGD-CBD	5.19	120.48	111.27
28	S	612	CLA	CMD-C2D-C1D	5.18	133.84	124.71
28	B	608	CLA	O2A-C1-C2	5.18	122.24	108.64
28	G	613	CLA	CMD-C2D-C1D	5.18	133.83	124.71
43	H	101	RRX	C24-C23-C22	5.17	134.05	126.23
28	b	617	CLA	O2A-C1-C2	5.17	122.22	108.64
47	N	620	LUT	C21-C26-C25	5.17	120.68	111.42
28	b	616	CLA	O2D-CGD-CBD	5.17	120.45	111.27
28	S	614	CLA	O2D-CGD-CBD	5.17	120.45	111.27
28	S	603	CLA	CMD-C2D-C1D	5.17	133.82	124.71
28	Y	612	CLA	O2D-CGD-CBD	5.16	120.44	111.27
28	B	604	CLA	O2A-C1-C2	5.15	122.17	108.64
28	d	403	CLA	O2A-C1-C2	5.15	122.16	108.64
28	Y	612	CLA	CMD-C2D-C1D	5.15	133.78	124.71
41	D	405	PL9	C7-C3-C4	5.14	121.06	116.88
28	A	407	CLA	O2A-C1-C2	5.14	122.15	108.64
28	B	616	CLA	O2D-CGD-CBD	5.14	120.40	111.27
28	N	611	CLA	O2A-C1-C2	5.13	120.97	108.97
28	N	614	CLA	O2D-CGD-CBD	5.13	120.39	111.27
28	c	512	CLA	O2A-C1-C2	5.13	122.12	108.64
28	b	607	CLA	O2D-CGD-CBD	5.13	120.39	111.27
28	B	612	CLA	O2A-C1-C2	5.13	122.11	108.64
28	a	410	CLA	O2D-CGD-CBD	5.13	120.38	111.27
28	c	502	CLA	O2A-C1-C2	5.13	122.11	108.64
28	d	402	CLA	O2D-CGD-CBD	5.13	120.38	111.27
28	B	604	CLA	O2D-CGD-CBD	5.12	120.37	111.27
28	C	511	CLA	O2D-CGD-CBD	5.12	120.37	111.27
28	c	505	CLA	CMD-C2D-C1D	5.12	133.73	124.71
30	c	516	BCR	C15-C14-C13	-5.11	120.02	127.31
47	S	620	LUT	C21-C26-C25	5.11	120.56	111.42
28	C	508	CLA	CMD-C2D-C1D	5.10	133.71	124.71
28	B	606	CLA	O2D-CGD-CBD	5.10	120.34	111.27
28	C	508	CLA	O2A-C1-C2	5.10	122.04	108.64
28	B	603	CLA	O2D-CGD-CBD	5.10	120.33	111.27
28	b	616	CLA	O2A-C1-C2	5.10	122.03	108.64
28	S	617	CLA	O2A-C1-C2	5.10	122.03	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	604	CLA	O2A-C1-C2	5.09	120.88	108.97
28	N	603	CLA	O2A-C1-C2	5.09	122.02	108.64
28	C	504	CLA	O2D-CGD-CBD	5.09	120.32	111.27
28	G	603	CLA	O2D-CGD-CBD	5.09	120.32	111.27
28	c	506	CLA	O2D-CGD-CBD	5.09	120.32	111.27
28	c	501	CLA	O2D-CGD-CBD	5.09	120.30	111.27
28	b	609	CLA	CMD-C2D-C1D	5.08	133.66	124.71
28	Y	611	CLA	O2D-CGD-CBD	5.08	120.29	111.27
28	C	510	CLA	O2A-C1-C2	5.08	121.98	108.64
28	c	510	CLA	O2D-CGD-CBD	5.07	120.29	111.27
28	S	612	CLA	O2D-CGD-CBD	5.07	120.27	111.27
28	C	502	CLA	O2D-CGD-CBD	5.06	120.27	111.27
43	H	101	RRX	C23-C22-C21	-5.06	111.18	118.94
28	Y	614	CLA	O2D-CGD-CBD	5.06	120.26	111.27
28	S	611	CLA	CMD-C2D-C1D	5.06	133.62	124.71
28	b	607	CLA	O2A-C1-C2	5.06	121.92	108.64
28	b	609	CLA	O2A-C1-C2	5.05	121.92	108.64
28	S	603	CLA	O2A-C1-C2	5.05	121.91	108.64
28	B	611	CLA	O2A-C1-C2	5.05	121.90	108.64
28	b	612	CLA	O2D-CGD-CBD	5.04	120.22	111.27
28	b	603	CLA	O2D-CGD-CBD	5.03	120.21	111.27
28	C	505	CLA	O2D-CGD-CBD	5.03	120.21	111.27
28	c	513	CLA	O2D-CGD-CBD	5.03	120.21	111.27
28	N	610	CLA	O2D-CGD-CBD	5.02	120.19	111.27
28	C	510	CLA	O2D-CGD-CBD	5.02	120.18	111.27
28	b	611	CLA	O2A-C1-C2	5.01	121.79	108.64
28	c	509	CLA	O2D-CGD-CBD	5.00	120.16	111.27
28	c	502	CLA	O2D-CGD-CBD	5.00	120.16	111.27
28	S	610	CLA	O2D-CGD-CBD	5.00	120.15	111.27
28	c	508	CLA	O2A-C1-C2	4.99	121.75	108.64
28	Y	604	CLA	O2A-C1-C2	4.99	121.75	108.64
28	b	606	CLA	O2D-CGD-CBD	4.99	120.13	111.27
28	c	503	CLA	O2D-CGD-CBD	4.99	120.13	111.27
28	C	512	CLA	O2A-C1-C2	4.98	121.73	108.64
28	d	402	CLA	CMD-C2D-C1D	4.98	133.49	124.71
28	b	602	CLA	O2A-C1-C2	4.98	121.72	108.64
28	S	611	CLA	O2A-C1-C2	4.98	121.71	108.64
28	c	503	CLA	O2A-C1-C2	4.96	121.68	108.64
28	c	512	CLA	CMD-C2D-C1D	4.96	133.46	124.71
34	b	620	C7Z	C35-C34-C33	-4.96	120.23	127.31
28	S	613	CLA	O2A-C1-C2	4.96	121.66	108.64
28	Y	611	CLA	O2A-C1-C2	4.96	121.66	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Y	602	CLA	O2A-C1-C2	4.95	121.66	108.64
28	D	402	CLA	CMD-C2D-C1D	4.95	133.44	124.71
28	C	507	CLA	O2D-CGD-CBD	4.94	120.05	111.27
28	b	604	CLA	O2D-CGD-CBD	4.94	120.05	111.27
28	b	605	CLA	O2D-CGD-CBD	4.94	120.04	111.27
47	N	621	LUT	C21-C26-C27	4.93	118.94	112.70
28	A	410	CLA	O2A-C1-C2	4.93	121.58	108.64
28	D	402	CLA	O2D-CGD-CBD	4.92	120.02	111.27
28	b	615	CLA	O2A-C1-C2	4.92	121.56	108.64
34	b	620	C7Z	C31-C30-C29	-4.92	120.30	127.31
28	N	602	CLA	O2A-C1-C2	4.91	121.54	108.64
28	G	602	CLA	CMD-C2D-C1D	4.90	133.35	124.71
28	B	612	CLA	CMD-C2D-C1D	4.89	133.34	124.71
28	c	511	CLA	O2D-CGD-CBD	4.89	119.96	111.27
28	C	501	CLA	O2A-C1-C2	4.89	121.49	108.64
43	H	101	RRX	C37-C22-C23	4.89	125.78	118.08
28	G	611	CLA	O2A-C1-C2	4.89	121.48	108.64
28	S	614	CLA	O2A-C1-C2	4.88	121.47	108.64
28	c	510	CLA	O2A-C1-C2	4.88	121.47	108.64
28	B	616	CLA	O2A-C1-C2	4.88	121.47	108.64
49	Y	623	NEX	C2-C1-C6	4.88	113.95	109.21
28	N	611	CLA	O2D-CGD-CBD	4.88	119.94	111.27
28	c	504	CLA	O2D-CGD-CBD	4.88	119.94	111.27
28	B	614	CLA	O2A-C1-C2	4.87	121.43	108.64
28	b	605	CLA	O2A-C1-C2	4.86	121.41	108.64
28	N	612	CLA	O2D-CGD-CBD	4.85	119.89	111.27
28	C	505	CLA	CMD-C2D-C1D	4.85	133.26	124.71
28	D	403	CLA	O2A-C1-C2	4.84	121.36	108.64
28	C	503	CLA	O2A-C1-C2	4.84	121.36	108.64
28	G	610	CLA	O2D-CGD-CBD	4.84	119.87	111.27
28	c	507	CLA	O2D-CGD-CBD	4.84	119.87	111.27
48	G	622	XAT	C31-C30-C29	-4.84	120.41	127.31
28	S	617	CLA	O2D-CGD-CBD	4.83	119.86	111.27
28	Y	610	CLA	O2D-CGD-CBD	4.83	119.86	111.27
28	b	602	CLA	O2D-CGD-CBD	4.83	119.85	111.27
28	Y	603	CLA	O2A-C1-C2	4.83	121.33	108.64
28	b	613	CLA	CMD-C2D-C1D	4.83	133.22	124.71
35	b	623	DGD	O2G-C1B-C2B	4.83	121.90	111.50
51	Y	627	PTY	O7-C8-C11	4.82	119.97	111.09
43	h	101	RRX	C24-C23-C22	4.82	133.53	126.23
28	Y	613	CLA	O2A-C1-C2	4.82	121.30	108.64
49	Y	623	NEX	C38-C25-C24	4.82	119.70	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	611	CLA	O2D-CGD-CBD	4.81	119.82	111.27
47	Y	621	LUT	C21-C26-C27	4.81	118.78	112.70
28	Y	608	CLA	O2D-CGD-CBD	4.81	119.81	111.27
28	B	608	CLA	O2D-CGD-CBD	4.80	119.80	111.27
28	b	614	CLA	O2A-C1-C2	4.80	121.24	108.64
28	c	513	CLA	O2A-C1-C2	4.80	121.24	108.64
28	C	511	CLA	O2A-C1-C2	4.79	121.23	108.64
28	Y	612	CLA	O2A-C1-C2	4.79	121.22	108.64
28	c	501	CLA	O2A-C1-C2	4.78	121.21	108.64
28	B	609	CLA	O2A-C1-C2	4.78	121.21	108.64
28	S	609	CLA	O2A-C1-C2	4.78	121.19	108.64
28	N	610	CLA	O2A-C1-C2	4.77	121.18	108.64
28	B	613	CLA	O2A-C1-C2	4.77	121.18	108.64
28	B	615	CLA	O2D-CGD-CBD	4.76	119.73	111.27
28	b	615	CLA	O2D-CGD-CBD	4.75	119.71	111.27
28	A	406	CLA	O2A-C1-C2	4.75	121.12	108.64
28	b	608	CLA	O2D-CGD-CBD	4.75	119.70	111.27
28	S	610	CLA	O2A-C1-C2	4.74	121.10	108.64
28	G	613	CLA	O2D-CGD-CBD	4.74	119.68	111.27
28	b	612	CLA	CMD-C2D-C1D	4.73	133.04	124.71
28	b	604	CLA	O2A-C1-C2	4.71	121.02	108.64
48	Y	622	XAT	C15-C14-C13	-4.71	120.59	127.31
49	S	623	NEX	C38-C25-C24	4.70	119.57	114.28
43	H	101	RRX	C21-C20-C19	-4.70	108.55	123.22
28	Y	614	CLA	O2A-C1-C2	4.69	120.96	108.64
28	B	615	CLA	O2A-C1-C2	4.69	120.96	108.64
28	b	617	CLA	CMD-C2D-C1D	4.68	132.96	124.71
28	b	614	CLA	O2D-CGD-CBD	4.66	119.56	111.27
28	B	610	CLA	CMD-C2D-C1D	4.65	132.90	124.71
28	C	508	CLA	O2D-CGD-CBD	4.64	119.52	111.27
43	h	101	RRX	C37-C22-C23	4.64	125.39	118.08
28	B	610	CLA	O2A-C1-C2	4.64	120.82	108.64
28	B	602	CLA	O2A-C1-C2	4.64	120.82	108.64
28	B	614	CLA	O2D-CGD-CBD	4.63	119.50	111.27
28	Y	613	CLA	O2D-CGD-CBD	4.63	119.50	111.27
28	c	506	CLA	O2A-C1-C2	4.63	120.80	108.64
28	a	405	CLA	O2A-C1-C2	4.63	120.79	108.64
28	N	613	CLA	O2D-CGD-CBD	4.63	119.49	111.27
28	C	512	CLA	CMD-C2D-C1D	4.62	132.86	124.71
30	c	514	BCR	C15-C14-C13	-4.62	120.71	127.31
28	B	617	CLA	CMD-C2D-C1D	4.62	132.86	124.71
28	B	610	CLA	O2D-CGD-CBD	4.61	119.46	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	G	623	NEX	C38-C25-C24	4.61	119.46	114.28
34	B	620	C7Z	C7-C8-C9	-4.60	119.29	126.23
43	h	101	RRX	C24-C25-C26	-4.59	110.35	121.46
28	Y	608	CLA	O2A-C1-C2	4.58	120.68	108.64
28	b	613	CLA	O2A-C1-C2	4.58	120.67	108.64
38	S	624	LHG	O7-C7-C8	4.56	121.33	111.50
32	W	201	LMG	O7-C10-C11	4.56	121.33	111.50
30	C	516	BCR	C33-C5-C6	-4.55	119.42	124.53
28	S	613	CLA	O2D-CGD-CBD	4.55	119.35	111.27
34	B	620	C7Z	C35-C34-C33	-4.53	120.84	127.31
48	G	622	XAT	C18-C5-C4	4.51	119.35	114.28
32	B	622	LMG	O7-C10-C11	4.50	121.20	111.50
48	N	622	XAT	C18-C5-C4	4.49	119.33	114.28
48	Y	622	XAT	C18-C5-C4	4.49	119.33	114.28
28	A	405	CLA	O2D-CGD-CBD	4.48	119.24	111.27
28	a	410	CLA	O2A-C1-C2	4.46	120.37	108.64
28	c	508	CLA	O2D-CGD-CBD	4.46	119.20	111.27
32	b	622	LMG	O7-C10-C11	4.46	121.11	111.50
43	h	101	RRX	C33-C5-C6	-4.45	119.53	124.53
28	A	405	CLA	O2A-C1-C2	4.44	120.31	108.64
47	S	620	LUT	C35-C34-C33	-4.43	120.99	127.31
30	c	516	BCR	C33-C5-C6	-4.41	119.57	124.53
34	b	620	C7Z	C7-C8-C9	-4.39	119.59	126.23
28	b	610	CLA	O2D-CGD-CBD	4.38	119.06	111.27
47	G	621	LUT	C35-C34-C33	-4.38	121.06	127.31
47	Y	620	LUT	C21-C26-C27	4.36	118.22	112.70
34	B	620	C7Z	C18-C5-C6	-4.36	119.63	124.53
32	A	413	LMG	O7-C10-C11	4.36	120.90	111.50
28	C	506	CLA	O2A-C1-C2	4.36	120.09	108.64
49	S	623	NEX	C2-C1-C6	4.35	113.43	109.21
48	G	622	XAT	C38-C25-C24	4.32	119.14	114.28
28	a	406	CLA	O2D-CGD-CBD	4.32	118.95	111.27
28	a	405	CLA	O2D-CGD-CBD	4.31	118.93	111.27
34	b	620	C7Z	C11-C10-C9	-4.31	121.17	127.31
38	N	624	LHG	O7-C7-C8	4.30	120.78	111.50
47	N	620	LUT	C21-C26-C27	4.30	118.14	112.70
34	B	620	C7Z	C1-C6-C5	-4.29	116.56	122.61
36	t	101	3PH	O21-C21-C22	4.29	120.75	111.50
43	H	101	RRX	C7-C8-C9	-4.29	119.75	126.23
43	h	101	RRX	C23-C22-C21	-4.28	112.38	118.94
43	h	101	RRX	C7-C8-C9	4.26	132.68	126.23
47	S	620	LUT	C21-C26-C27	4.26	118.09	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N	622	XAT	O24-C25-C24	4.24	116.57	113.38
48	N	622	XAT	C38-C25-C24	4.23	119.04	114.28
47	G	620	LUT	C15-C14-C13	-4.22	121.28	127.31
32	C	521	LMG	O7-C10-C11	4.22	120.60	111.50
47	N	621	LUT	C22-C23-C24	-4.22	106.94	111.74
38	d	410	LHG	O7-C7-C8	4.21	120.58	111.50
43	h	101	RRX	C21-C20-C19	-4.21	110.07	123.22
47	G	620	LUT	C21-C26-C27	4.19	118.00	112.70
47	N	621	LUT	C35-C34-C33	-4.18	121.34	127.31
34	B	620	C7Z	C38-C25-C26	-4.18	119.83	124.53
34	b	620	C7Z	C1-C6-C5	-4.18	116.73	122.61
48	Y	622	XAT	C38-C25-C24	4.17	118.97	114.28
49	N	623	NEX	C38-C25-C24	4.16	118.97	114.28
28	A	406	CLA	O2D-CGD-CBD	4.16	118.66	111.27
47	S	621	LUT	C21-C26-C27	4.15	117.95	112.70
47	N	621	LUT	C7-C8-C9	-4.15	119.96	126.23
32	H	102	LMG	O7-C10-C11	4.13	120.41	111.50
43	h	101	RRX	C34-C9-C8	4.13	124.58	118.08
32	h	102	LMG	O7-C10-C11	4.11	120.37	111.50
47	Y	621	LUT	C22-C23-C24	-4.11	107.06	111.74
43	h	101	RRX	C15-C14-C13	-4.08	121.49	127.31
38	C	525	LHG	O7-C7-C8	4.07	120.28	111.50
48	Y	622	XAT	C7-C8-C9	-4.07	119.22	125.53
38	D	410	LHG	O7-C7-C8	4.06	120.26	111.50
38	c	525	LHG	O7-C7-C8	4.05	120.24	111.50
32	C	523	LMG	O7-C10-C11	4.05	120.23	111.50
30	B	618	BCR	C15-C14-C13	-4.05	121.53	127.31
32	c	523	LMG	O7-C10-C11	4.04	120.20	111.50
30	b	618	BCR	C27-C26-C25	-4.04	116.87	122.73
47	N	620	LUT	C15-C14-C13	-4.02	121.57	127.31
37	b	625	DGA	OG2-CB1-CB2	4.02	120.16	111.50
34	b	620	C7Z	C27-C28-C29	-4.02	120.17	126.23
38	G	624	LHG	O7-C7-C8	4.01	120.14	111.50
46	Y	609	CHL	CHD-C1D-ND	-4.00	120.78	124.45
36	B	624	3PH	O21-C21-C22	3.99	120.10	111.50
46	G	609	CHL	CHD-C1D-ND	-3.99	120.79	124.45
38	Y	624	LHG	O7-C7-C8	3.99	120.09	111.50
32	a	413	LMG	O7-C10-C11	3.99	120.09	111.50
48	Y	622	XAT	C36-C21-C26	3.98	120.79	110.05
38	D	409	LHG	O7-C7-C8	3.97	120.05	111.50
30	A	411	BCR	C33-C5-C6	-3.96	120.08	124.53
47	G	620	LUT	C22-C23-C24	-3.96	107.23	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	Y	621	LUT	C35-C34-C33	-3.95	121.67	127.31
47	G	621	LUT	C22-C23-C24	-3.94	107.26	111.74
37	B	625	DGA	OG2-CB1-CB2	3.94	119.98	111.50
36	b	624	3PH	O21-C21-C22	3.93	119.98	111.50
28	C	509	CLA	O2A-C1-C2	3.91	118.91	108.64
37	c	524	DGA	OG2-CB1-CB2	3.91	119.93	111.50
51	Y	626	PTY	O7-C8-C11	3.91	119.92	111.50
28	c	507	CLA	C2C-C1C-NC	3.91	113.63	109.97
47	S	621	LUT	C22-C23-C24	-3.91	107.30	111.74
37	J	101	DGA	OG2-CB1-CB2	3.90	119.90	111.50
37	C	524	DGA	OG2-CB1-CB2	3.88	119.87	111.50
28	b	612	CLA	C1-C2-C3	-3.88	119.34	126.04
30	b	618	BCR	C15-C14-C13	-3.87	121.79	127.31
35	C	519	DGD	O2G-C1B-C2B	3.86	119.83	111.50
38	d	409	LHG	O7-C7-C8	3.86	119.81	111.50
47	G	621	LUT	C7-C8-C9	-3.85	120.42	126.23
47	S	621	LUT	C35-C34-C33	-3.85	121.82	127.31
46	G	601	CHL	CHD-C1D-ND	-3.85	120.92	124.45
46	Y	601	CHL	CHD-C1D-ND	-3.84	120.92	124.45
49	G	623	NEX	C17-C1-C6	-3.83	107.05	110.47
28	b	611	CLA	C2D-C1D-ND	3.82	112.92	110.10
32	w	201	LMG	O7-C10-C11	3.80	119.70	111.50
28	A	406	CLA	C2C-C1C-NC	3.79	113.52	109.97
32	D	411	LMG	O7-C10-C11	3.78	119.66	111.50
47	Y	620	LUT	C22-C23-C24	-3.78	107.44	111.74
48	G	622	XAT	O24-C25-C24	3.78	116.22	113.38
36	T	101	3PH	O21-C21-C22	3.78	119.64	111.50
38	D	408	LHG	O7-C7-C8	3.78	119.64	111.50
45	i	101	4RF	O21-C22-C24	3.77	119.62	111.50
45	I	102	4RF	O21-C22-C24	3.77	119.62	111.50
47	S	620	LUT	C7-C8-C9	-3.76	120.55	126.23
45	k	101	4RF	O21-C22-C24	3.76	119.60	111.50
28	B	605	CLA	C2C-C1C-NC	3.75	113.49	109.97
47	N	621	LUT	C15-C14-C13	-3.75	121.96	127.31
47	Y	621	LUT	C7-C8-C9	-3.75	120.57	126.23
43	H	101	RRX	C33-C5-C6	-3.74	120.33	124.53
28	B	606	CLA	CHD-C1D-ND	-3.74	121.02	124.45
37	j	101	DGA	OG2-CB1-CB2	3.73	119.53	111.50
28	c	509	CLA	O2A-C1-C2	3.72	118.42	108.64
30	B	618	BCR	C1-C6-C5	-3.70	117.40	122.61
47	G	620	LUT	C35-C34-C33	-3.70	122.03	127.31
28	B	605	CLA	C1-C2-C3	-3.69	119.65	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	N	613	CLA	CMA-C3A-C4A	3.69	121.69	111.77
47	N	620	LUT	C35-C34-C33	-3.69	122.04	127.31
46	G	605	CHL	C2C-C3C-C4C	3.68	109.11	106.49
46	N	601	CHL	CHD-C1D-ND	-3.67	121.08	124.45
35	c	518	DGD	O2G-C1B-C2B	3.67	119.42	111.50
30	b	618	BCR	C33-C5-C6	-3.67	120.40	124.53
28	c	502	CLA	C2C-C1C-NC	3.67	113.41	109.97
39	c	527	LMK	O3-C4-C3	-3.67	110.40	122.98
28	b	605	CLA	CMA-C3A-C4A	3.67	121.63	111.77
49	S	623	NEX	C27-C28-C29	-3.67	119.84	125.53
49	S	623	NEX	C16-C1-C6	-3.66	107.19	110.47
35	C	518	DGD	O2G-C1B-C2B	3.66	119.39	111.50
30	c	515	BCR	C33-C5-C6	-3.66	120.42	124.53
28	b	609	CLA	C1-C2-C3	-3.66	119.71	126.04
28	G	603	CLA	C1-C2-C3	-3.66	119.72	126.04
28	c	504	CLA	C2C-C1C-NC	3.66	113.40	109.97
28	a	405	CLA	C2D-C1D-ND	3.66	112.80	110.10
49	G	623	NEX	C27-C28-C29	-3.65	119.86	125.53
31	m	101	SQD	O7-S-C6	-3.65	102.61	106.94
46	N	608	CHL	CHD-C1D-ND	-3.65	121.10	124.45
35	C	520	DGD	O2G-C1B-C2B	3.64	119.34	111.50
41	d	405	PL9	C7-C3-C2	-3.64	118.52	123.30
47	G	621	LUT	C15-C14-C13	-3.64	122.12	127.31
32	d	411	LMG	O7-C10-C11	3.63	119.33	111.50
43	H	101	RRX	C15-C16-C17	-3.63	116.04	123.47
43	H	101	RRX	C1-C6-C5	-3.63	117.50	122.61
31	a	412	SQD	O7-S-C6	-3.63	102.63	106.94
29	a	409	PHO	CMB-C2B-C3B	3.62	131.45	124.68
28	S	617	CLA	C1-C2-C3	-3.61	120.90	126.75
28	G	613	CLA	C1-C2-C3	-3.60	119.81	126.04
28	C	508	CLA	C1-C2-C3	-3.60	119.82	126.04
47	S	621	LUT	C7-C8-C9	-3.60	120.80	126.23
28	b	609	CLA	CMB-C2B-C3B	3.59	131.40	124.68
28	c	505	CLA	C1-C2-C3	-3.59	119.83	126.04
28	G	611	CLA	C2C-C1C-NC	3.59	113.34	109.97
28	C	513	CLA	C2D-C1D-ND	3.59	112.75	110.10
45	K	101	4RF	O21-C22-C24	3.59	119.24	111.50
30	a	411	BCR	C33-C5-C6	-3.59	120.50	124.53
31	B	626	SQD	O7-S-C6	-3.59	102.68	106.94
30	B	618	BCR	C33-C5-C4	3.59	120.50	113.62
30	c	517	BCR	C33-C5-C4	3.59	120.50	113.62
47	N	620	LUT	C22-C23-C24	-3.58	107.66	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	521	LMG	O7-C10-C11	3.58	119.22	111.50
28	b	606	CLA	CHD-C1D-ND	-3.58	121.16	124.45
28	c	509	CLA	C2C-C1C-NC	3.58	113.32	109.97
46	S	606	CHL	CHD-C1D-ND	-3.58	121.17	124.45
31	C	526	SQD	O7-S-C6	-3.57	102.69	106.94
28	b	605	CLA	C2C-C1C-NC	3.57	113.32	109.97
28	S	605	CLA	C2C-C1C-NC	3.57	113.32	109.97
31	M	101	SQD	O7-S-C6	-3.57	102.70	106.94
31	b	621	SQD	O7-S-C6	-3.56	102.70	106.94
46	Y	606	CHL	CHD-C1D-ND	-3.56	121.18	124.45
47	Y	621	LUT	C11-C10-C9	-3.55	122.25	127.31
28	Y	608	CLA	C1-C2-C3	-3.55	121.01	126.75
47	N	621	LUT	C18-C5-C6	-3.55	120.55	124.53
28	C	509	CLA	C2C-C1C-NC	3.54	113.29	109.97
28	B	611	CLA	C2C-C1C-NC	3.54	113.29	109.97
47	S	621	LUT	C18-C5-C6	-3.54	120.55	124.53
28	G	603	CLA	C2C-C1C-NC	3.54	113.29	109.97
31	b	626	SQD	O7-S-C6	-3.54	102.73	106.94
30	B	618	BCR	C33-C5-C6	-3.54	120.56	124.53
28	a	406	CLA	O2A-C1-C2	3.54	117.93	108.64
47	Y	620	LUT	C35-C34-C33	-3.54	122.26	127.31
46	S	607	CHL	CHD-C1D-ND	-3.54	121.20	124.45
47	Y	621	LUT	C15-C14-C13	-3.53	122.27	127.31
35	c	520	DGD	O2G-C1B-C2B	3.53	119.12	111.50
28	A	405	CLA	CMB-C2B-C3B	3.53	131.29	124.68
28	c	503	CLA	C1-C2-C3	-3.53	119.93	126.04
47	Y	620	LUT	C15-C14-C13	-3.53	122.28	127.31
31	A	412	SQD	O7-S-C6	-3.52	102.75	106.94
47	Y	620	LUT	C7-C8-C9	-3.52	120.91	126.23
47	N	621	LUT	C11-C10-C9	-3.51	122.30	127.31
48	G	622	XAT	C7-C8-C9	-3.50	120.09	125.53
28	G	610	CLA	C1-C2-C3	-3.50	119.98	126.04
38	d	408	LHG	O7-C7-C8	3.50	119.05	111.50
28	b	603	CLA	C1-C2-C3	-3.50	119.99	126.04
28	G	614	CLA	CHD-C1D-ND	-3.49	121.25	124.45
31	B	621	SQD	O7-S-C6	-3.49	102.79	106.94
31	c	526	SQD	O7-S-C6	-3.49	102.79	106.94
28	S	605	CLA	C1-C2-C3	-3.48	121.11	126.75
49	N	623	NEX	C5-C4-C3	3.48	115.87	111.75
28	d	403	CLA	C1-C2-C3	-3.48	120.02	126.04
28	S	611	CLA	C2C-C1C-NC	3.48	113.23	109.97
28	D	402	CLA	C1-C2-C3	-3.48	120.03	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	D	405	PL9	C7-C3-C2	-3.48	118.73	123.30
28	C	510	CLA	C1C-C2C-C3C	-3.47	103.30	106.96
49	N	623	NEX	C27-C28-C29	-3.47	120.15	125.53
28	S	613	CLA	C1-C2-C3	-3.46	120.05	126.04
28	S	603	CLA	C2C-C1C-NC	3.46	113.21	109.97
28	N	604	CLA	C1-C2-C3	-3.45	120.07	126.04
28	b	611	CLA	C2C-C1C-NC	3.45	113.21	109.97
28	b	615	CLA	CHD-C1D-ND	-3.45	121.28	124.45
30	b	618	BCR	C33-C5-C4	3.45	120.24	113.62
46	N	605	CHL	CHD-C1D-ND	-3.45	121.28	124.45
46	G	605	CHL	CHD-C1D-ND	-3.45	121.29	124.45
43	H	101	RRX	C4-C5-C6	-3.44	117.74	122.73
28	C	508	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
28	A	406	CLA	C1-C2-C3	-3.43	120.10	126.04
43	h	101	RRX	C1-C6-C5	-3.43	117.78	122.61
30	c	517	BCR	C37-C22-C21	-3.43	118.12	122.92
28	C	506	CLA	C2C-C1C-NC	3.43	113.18	109.97
28	A	410	CLA	CMB-C2B-C3B	3.42	131.08	124.68
34	b	620	C7Z	C18-C5-C4	3.42	120.69	114.36
46	S	601	CHL	CHD-C1D-ND	-3.42	121.31	124.45
47	G	621	LUT	C11-C10-C9	-3.41	122.44	127.31
28	C	501	CLA	CHD-C1D-ND	-3.41	121.32	124.45
28	b	614	CLA	C2C-C1C-NC	3.41	113.17	109.97
46	G	606	CHL	CHD-C1D-ND	-3.41	121.32	124.45
28	a	405	CLA	CHD-C1D-ND	-3.41	121.32	124.45
28	c	512	CLA	C2C-C1C-NC	3.40	113.16	109.97
49	Y	623	NEX	C31-C30-C29	3.40	132.17	127.31
28	S	614	CLA	CHD-C1D-ND	-3.40	121.33	124.45
46	Y	605	CHL	CHD-C1D-ND	-3.40	121.33	124.45
28	C	507	CLA	C2C-C1C-NC	3.40	113.16	109.97
28	c	508	CLA	CHD-C1D-ND	-3.39	121.34	124.45
28	a	406	CLA	C2C-C1C-NC	3.39	113.15	109.97
28	c	511	CLA	C1-C2-C3	-3.39	120.19	126.04
28	c	504	CLA	C1-C2-C3	-3.38	120.19	126.04
28	A	405	CLA	C1-C2-C3	-3.38	120.19	126.04
35	c	519	DGD	O2G-C1B-C2B	3.38	118.78	111.50
28	C	510	CLA	C1-C2-C3	-3.37	120.21	126.04
46	G	601	CHL	C2C-C3C-C4C	3.37	108.89	106.49
28	c	513	CLA	CHD-C1D-ND	-3.37	121.36	124.45
28	S	604	CLA	C2C-C1C-NC	3.37	113.12	109.97
34	B	620	C7Z	C31-C30-C29	-3.36	122.52	127.31
28	C	508	CLA	CMB-C2B-C3B	3.36	130.96	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	620	C7Z	C18-C5-C6	-3.35	120.76	124.53
46	G	605	CHL	C3C-C4C-NC	-3.35	106.81	110.57
28	C	511	CLA	CHD-C1D-ND	-3.35	121.38	124.45
28	N	602	CLA	CHD-C1D-ND	-3.35	121.38	124.45
28	Y	612	CLA	C2C-C1C-NC	3.34	113.11	109.97
28	c	506	CLA	C2C-C1C-NC	3.34	113.10	109.97
49	Y	623	NEX	C27-C28-C29	-3.34	120.34	125.53
28	d	403	CLA	CHD-C1D-ND	-3.34	121.39	124.45
47	S	620	LUT	C35-C15-C14	-3.34	116.64	123.47
28	b	603	CLA	CHD-C1D-ND	-3.34	121.39	124.45
42	f	101	HEM	CMC-C2C-C3C	3.34	130.92	124.68
28	A	405	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
28	c	510	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
34	B	620	C7Z	C27-C28-C29	-3.33	121.20	126.23
46	S	608	CHL	CHD-C1D-ND	-3.33	121.39	124.45
28	c	510	CLA	CHD-C1D-ND	-3.33	121.39	124.45
28	B	606	CLA	C1-C2-C3	-3.33	120.28	126.04
46	G	607	CHL	CHD-C1D-ND	-3.33	121.39	124.45
28	c	508	CLA	CMB-C2B-C3B	3.33	130.91	124.68
30	c	515	BCR	C15-C14-C13	-3.33	122.56	127.31
28	c	510	CLA	C2D-C1D-ND	3.33	112.56	110.10
28	D	403	CLA	C2C-C1C-NC	3.33	113.09	109.97
48	G	622	XAT	C38-C25-C26	-3.32	116.69	122.26
28	C	510	CLA	CHD-C1D-ND	-3.32	121.40	124.45
28	C	501	CLA	CMA-C3A-C4A	3.32	120.70	111.77
46	N	607	CHL	CHD-C1D-ND	-3.32	121.40	124.45
47	S	620	LUT	C15-C14-C13	-3.32	122.57	127.31
28	A	407	CLA	C1-C2-C3	-3.32	121.39	126.75
28	a	410	CLA	CMB-C2B-C3B	3.31	130.88	124.68
28	A	407	CLA	C2C-C1C-NC	3.31	113.08	109.97
28	b	609	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
28	B	606	CLA	C2C-C1C-NC	3.31	113.07	109.97
46	N	609	CHL	CHD-C1D-ND	-3.30	121.42	124.45
28	c	503	CLA	CHD-C1D-ND	-3.30	121.42	124.45
28	B	615	CLA	C1-C2-C3	-3.30	120.33	126.04
46	G	601	CHL	C3C-C4C-NC	-3.30	106.87	110.57
46	N	601	CHL	C2C-C3C-C4C	3.30	108.84	106.49
47	G	620	LUT	C7-C8-C9	-3.30	121.25	126.23
30	c	517	BCR	C4-C5-C6	-3.30	117.94	122.73
28	c	508	CLA	C1-C2-C3	-3.29	120.34	126.04
28	G	610	CLA	CHD-C1D-ND	-3.29	121.43	124.45
28	S	602	CLA	C1-C2-C3	-3.29	120.35	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	501	CLA	C1-C2-C3	-3.29	120.36	126.04
28	N	612	CLA	C2C-C1C-NC	3.28	113.05	109.97
28	N	614	CLA	CHD-C1D-ND	-3.28	121.44	124.45
28	Y	610	CLA	C1-C2-C3	-3.28	120.37	126.04
28	b	602	CLA	C2C-C1C-NC	3.28	113.04	109.97
48	N	622	XAT	C6-C7-C8	-3.27	119.07	125.99
28	G	603	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
30	B	619	BCR	C33-C5-C6	-3.27	120.86	124.53
28	c	507	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
28	S	613	CLA	CMA-C3A-C4A	3.27	120.56	111.77
28	N	602	CLA	C1-C2-C3	-3.27	120.39	126.04
46	S	606	CHL	C2C-C3C-C4C	3.27	108.82	106.49
28	G	612	CLA	C2C-C1C-NC	3.27	113.03	109.97
28	Y	610	CLA	CHD-C1D-ND	-3.26	121.45	124.45
30	B	619	BCR	C33-C5-C4	3.26	119.89	113.62
28	a	406	CLA	CMB-C2B-C3B	3.26	130.78	124.68
28	G	602	CLA	C2C-C1C-NC	3.26	113.03	109.97
28	B	607	CLA	CHD-C1D-ND	-3.26	121.46	124.45
28	Y	613	CLA	CHD-C1D-ND	-3.26	121.46	124.45
28	B	609	CLA	C1-C2-C3	-3.26	120.41	126.04
28	A	410	CLA	CHD-C1D-ND	-3.26	121.46	124.45
28	B	614	CLA	C2C-C1C-NC	3.26	113.02	109.97
28	c	511	CLA	CMA-C3A-C4A	3.25	120.52	111.77
28	S	617	CLA	C2C-C1C-NC	3.25	113.02	109.97
28	c	501	CLA	C1-C2-C3	-3.25	120.42	126.04
46	G	608	CHL	CHD-C1D-ND	-3.25	121.47	124.45
28	B	603	CLA	CHD-C1D-ND	-3.25	121.47	124.45
28	B	602	CLA	C2C-C1C-NC	3.25	113.02	109.97
28	C	502	CLA	C2C-C1C-NC	3.25	113.02	109.97
46	Y	606	CHL	C2C-C3C-C4C	3.25	108.81	106.49
28	b	616	CLA	C1-C2-C3	-3.25	120.42	126.04
46	S	607	CHL	C2C-C3C-C4C	3.25	108.80	106.49
49	G	623	NEX	C20-C13-C14	-3.25	118.38	122.92
40	d	401	BCT	O3-C-O1	-3.24	111.14	119.55
28	S	604	CLA	CHD-C1D-ND	-3.24	121.48	124.45
43	H	101	RRX	C33-C5-C4	3.24	119.84	113.62
28	D	403	CLA	CHD-C1D-ND	-3.24	121.48	124.45
30	c	514	BCR	C33-C5-C6	-3.24	120.89	124.53
47	S	620	LUT	C18-C5-C6	-3.24	120.89	124.53
46	N	605	CHL	C2C-C3C-C4C	3.23	108.80	106.49
28	B	614	CLA	CHD-C1D-ND	-3.23	121.48	124.45
28	a	407	CLA	C2D-C1D-ND	3.23	112.48	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	608	CLA	C2C-C1C-NC	3.22	112.99	109.97
30	a	411	BCR	C33-C5-C4	3.22	119.80	113.62
28	C	502	CLA	C1-C2-C3	-3.22	120.48	126.04
28	N	611	CLA	C2C-C1C-NC	3.22	112.98	109.97
28	c	512	CLA	CMB-C2B-C3B	3.22	130.69	124.68
28	N	603	CLA	C1-C2-C3	-3.21	120.49	126.04
46	Y	609	CHL	CMA-C3A-C4A	3.21	120.40	111.77
28	b	612	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
28	C	510	CLA	C2C-C1C-NC	3.20	112.97	109.97
30	C	514	BCR	C33-C5-C6	-3.20	120.93	124.53
49	G	623	NEX	C39-C29-C30	-3.20	118.44	122.92
28	C	503	CLA	CMA-C3A-C4A	3.20	120.38	111.77
28	S	611	CLA	C1-C2-C3	-3.20	120.51	126.04
28	B	617	CLA	C2C-C1C-NC	3.20	112.97	109.97
28	B	609	CLA	C2C-C1C-NC	3.20	112.97	109.97
28	N	610	CLA	CHD-C1D-ND	-3.19	121.52	124.45
28	c	501	CLA	CHD-C1D-ND	-3.19	121.52	124.45
46	N	607	CHL	CHB-C4A-NA	3.19	128.93	124.51
28	C	508	CLA	CHD-C1D-ND	-3.19	121.52	124.45
28	b	607	CLA	CHD-C1D-ND	-3.19	121.52	124.45
46	Y	609	CHL	C3C-C4C-NC	-3.19	107.00	110.57
28	Y	614	CLA	C2C-C1C-NC	3.19	112.96	109.97
30	b	619	BCR	C15-C14-C13	-3.19	122.76	127.31
28	B	603	CLA	C2C-C1C-NC	3.19	112.96	109.97
28	N	614	CLA	C2C-C1C-NC	3.19	112.96	109.97
30	b	619	BCR	C33-C5-C4	3.19	119.74	113.62
28	Y	603	CLA	CHD-C1D-ND	-3.18	121.53	124.45
46	G	609	CHL	CMA-C3A-C4A	3.18	120.33	111.77
28	D	402	CLA	C2D-C1D-ND	3.18	112.45	110.10
28	Y	608	CLA	C2C-C1C-NC	3.18	112.95	109.97
28	C	512	CLA	C2C-C1C-NC	3.18	112.95	109.97
28	B	604	CLA	C2C-C1C-NC	3.17	112.94	109.97
30	C	517	BCR	C36-C18-C17	-3.17	118.48	122.92
28	S	610	CLA	CHD-C1D-ND	-3.17	121.54	124.45
28	S	603	CLA	CMA-C3A-C4A	3.17	120.29	111.77
28	b	610	CLA	CHD-C1D-ND	-3.17	121.54	124.45
28	B	615	CLA	CHD-C1D-ND	-3.16	121.55	124.45
28	B	605	CLA	CMA-C3A-C4A	3.16	120.27	111.77
28	N	603	CLA	C2C-C1C-NC	3.16	112.93	109.97
28	C	512	CLA	C2D-C1D-ND	3.16	112.43	110.10
46	N	606	CHL	C2C-C3C-C4C	3.16	108.74	106.49
28	b	604	CLA	C2C-C1C-NC	3.16	112.93	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	N	601	CHL	C3C-C4C-NC	-3.16	107.03	110.57
30	c	515	BCR	C33-C5-C4	3.15	119.68	113.62
28	B	611	CLA	C1-C2-C3	-3.15	120.59	126.04
48	N	622	XAT	C38-C25-C26	-3.15	116.98	122.26
30	B	619	BCR	C23-C24-C25	-3.15	118.35	127.20
28	B	613	CLA	C2C-C1C-NC	3.15	112.92	109.97
28	B	609	CLA	CHD-C1D-ND	-3.15	121.56	124.45
28	b	616	CLA	C2C-C1C-NC	3.15	112.92	109.97
46	N	607	CHL	C2C-C3C-C4C	3.15	108.73	106.49
28	A	405	CLA	CHD-C1D-ND	-3.15	121.56	124.45
28	c	503	CLA	C2D-C1D-ND	3.15	112.42	110.10
28	b	611	CLA	C1-C2-C3	-3.14	120.60	126.04
46	N	607	CHL	C3C-C4C-NC	-3.14	107.05	110.57
28	A	410	CLA	C2C-C1C-NC	3.14	112.91	109.97
28	C	505	CLA	C2C-C1C-NC	3.14	112.91	109.97
46	G	608	CHL	CMA-C3A-C4A	3.14	120.21	111.77
30	a	411	BCR	C38-C26-C25	-3.14	121.00	124.53
28	N	604	CLA	C2C-C1C-NC	3.14	112.91	109.97
28	b	606	CLA	C2C-C1C-NC	3.14	112.91	109.97
29	A	409	PHO	CMB-C2B-C3B	3.14	130.54	124.68
34	B	620	C7Z	C2-C3-C4	3.14	114.60	110.30
28	b	612	CLA	CMB-C2B-C3B	3.13	130.53	124.68
28	c	513	CLA	C1-C2-C3	-3.13	120.63	126.04
28	b	608	CLA	C2C-C1C-NC	3.13	112.90	109.97
28	S	613	CLA	C2C-C1C-NC	3.13	112.90	109.97
28	B	615	CLA	C2C-C1C-NC	3.13	112.90	109.97
46	S	606	CHL	C3C-C4C-NC	-3.12	107.07	110.57
28	c	503	CLA	CMA-C3A-C4A	3.12	120.16	111.77
28	C	506	CLA	CHD-C1D-ND	-3.12	121.59	124.45
28	Y	603	CLA	C2C-C1C-NC	3.12	112.89	109.97
46	S	608	CHL	CMA-C3A-C4A	3.11	120.14	111.77
46	S	601	CHL	C3C-C4C-NC	-3.11	107.09	110.57
28	S	603	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
46	Y	607	CHL	CHD-C1D-ND	-3.10	121.60	124.45
49	Y	623	NEX	C39-C29-C30	-3.10	118.58	122.92
46	N	605	CHL	C3C-C4C-NC	-3.10	107.09	110.57
46	N	609	CHL	CMA-C3A-C4A	3.10	120.10	111.77
46	S	601	CHL	C2C-C3C-C4C	3.10	108.70	106.49
28	b	603	CLA	C2C-C1C-NC	3.10	112.87	109.97
47	N	620	LUT	C11-C10-C9	-3.10	122.89	127.31
28	c	505	CLA	C2C-C1C-NC	3.09	112.87	109.97
46	S	607	CHL	CMA-C3A-C4A	3.09	120.07	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	N	613	CLA	C2C-C1C-NC	3.09	112.86	109.97
28	D	403	CLA	C1-C2-C3	-3.09	120.70	126.04
28	C	504	CLA	C1-C2-C3	-3.09	120.70	126.04
47	S	621	LUT	C38-C25-C24	-3.09	116.96	123.56
46	S	607	CHL	C3C-C4C-NC	-3.09	107.11	110.57
28	G	613	CLA	CMA-C3A-C4A	3.08	120.06	111.77
28	c	502	CLA	CMA-C3A-C4A	3.08	120.06	111.77
28	c	501	CLA	CMA-C3A-C4A	3.08	120.06	111.77
28	b	614	CLA	C1-C2-C3	-3.08	120.71	126.04
28	c	511	CLA	C2C-C1C-NC	3.08	112.86	109.97
28	b	611	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
28	a	407	CLA	CMA-C3A-C4A	3.08	120.06	111.77
28	C	513	CLA	CMD-C2D-C1D	3.08	130.14	124.71
28	S	612	CLA	C2D-C1D-ND	3.08	112.37	110.10
28	S	602	CLA	CHD-C1D-ND	-3.08	121.62	124.45
28	S	613	CLA	CHD-C1D-ND	-3.08	121.62	124.45
28	C	504	CLA	C2D-C1D-ND	3.08	112.37	110.10
28	Y	604	CLA	CHD-C1D-ND	-3.08	121.63	124.45
46	Y	606	CHL	C3C-C4C-NC	-3.08	107.12	110.57
28	Y	611	CLA	C2C-C1C-NC	3.08	112.85	109.97
28	c	508	CLA	C2D-C1D-ND	3.07	112.37	110.10
46	G	605	CHL	CMA-C3A-C4A	3.07	120.04	111.77
46	Y	609	CHL	C2C-C3C-C4C	3.07	108.68	106.49
28	b	602	CLA	CHD-C1D-ND	-3.07	121.63	124.45
28	a	405	CLA	C1-C2-C3	-3.07	120.73	126.04
28	a	410	CLA	C2C-C1C-NC	3.07	112.85	109.97
28	G	603	CLA	CHD-C1D-ND	-3.07	121.63	124.45
28	G	604	CLA	C2C-C1C-NC	3.07	112.84	109.97
28	c	502	CLA	CHD-C1D-ND	-3.07	121.64	124.45
28	Y	608	CLA	CHD-C1D-ND	-3.06	121.64	124.45
28	b	616	CLA	CHD-C1D-ND	-3.06	121.64	124.45
28	B	610	CLA	C2C-C1C-NC	3.06	112.84	109.97
28	B	616	CLA	C2C-C1C-NC	3.06	112.84	109.97
28	b	606	CLA	C2D-C1D-ND	3.06	112.36	110.10
28	N	613	CLA	O2A-CGA-CBA	3.06	121.51	111.91
30	d	404	BCR	C1-C6-C5	-3.06	118.31	122.61
28	c	504	CLA	CMA-C3A-C4A	3.06	119.99	111.77
28	S	612	CLA	CMB-C2B-C3B	3.06	130.40	124.68
30	D	404	BCR	C34-C9-C10	-3.06	118.64	122.92
49	Y	623	NEX	C17-C1-C6	-3.06	107.74	110.47
46	G	607	CHL	CMA-C3A-C4A	3.06	119.99	111.77
28	S	609	CLA	CHD-C1D-ND	-3.06	121.65	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	509	CLA	CHD-C1D-ND	-3.06	121.65	124.45
28	c	511	CLA	CHD-C1D-ND	-3.06	121.65	124.45
28	C	511	CLA	C2C-C1C-NC	3.06	112.83	109.97
46	S	606	CHL	CMA-C3A-C4A	3.05	119.98	111.77
28	c	510	CLA	C1-C2-C3	-3.05	120.76	126.04
46	Y	601	CHL	CMA-C3A-C4A	3.05	119.98	111.77
28	S	609	CLA	CMA-C3A-C4A	3.05	119.97	111.77
46	G	606	CHL	C2C-C3C-C4C	3.05	108.66	106.49
28	Y	614	CLA	CHD-C1D-ND	-3.05	121.65	124.45
46	N	601	CHL	CMA-C3A-C4A	3.05	119.96	111.77
46	Y	606	CHL	CMA-C3A-C4A	3.05	119.96	111.77
46	G	607	CHL	C4A-NA-C1A	3.05	108.08	106.71
28	G	602	CLA	CMA-C3A-C4A	3.04	119.96	111.77
28	b	617	CLA	C1-C2-C3	-3.04	120.78	126.04
28	b	607	CLA	C2C-C1C-NC	3.04	112.82	109.97
28	C	509	CLA	CHD-C1D-ND	-3.04	121.66	124.45
28	a	410	CLA	CMA-C3A-C4A	3.04	119.94	111.77
49	G	623	NEX	C31-C30-C29	3.03	131.64	127.31
46	Y	605	CHL	C3C-C4C-NC	-3.03	107.17	110.57
30	C	515	BCR	C33-C5-C6	-3.03	121.12	124.53
30	d	404	BCR	C4-C5-C6	-3.03	118.33	122.73
30	C	517	BCR	C37-C22-C21	-3.03	118.68	122.92
28	C	503	CLA	C2C-C1C-NC	3.03	112.81	109.97
28	b	609	CLA	C2C-C1C-NC	3.03	112.81	109.97
46	G	606	CHL	C3C-C4C-NC	-3.03	107.17	110.57
28	c	510	CLA	C2C-C1C-NC	3.03	112.81	109.97
28	Y	612	CLA	C2D-C1D-ND	3.03	112.33	110.10
28	B	602	CLA	C2D-C1D-ND	3.02	112.33	110.10
30	d	404	BCR	C33-C5-C4	3.02	119.42	113.62
28	C	513	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
28	B	614	CLA	C1-C2-C3	-3.02	120.82	126.04
28	A	406	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
30	C	514	BCR	C15-C14-C13	-3.02	123.00	127.31
28	S	612	CLA	C2C-C1C-NC	3.02	112.80	109.97
28	A	407	CLA	CMA-C3A-C4A	3.02	119.89	111.77
28	G	611	CLA	CMA-C3A-C4A	3.02	119.88	111.77
28	B	603	CLA	C1-C2-C3	-3.02	120.83	126.04
28	S	609	CLA	C2C-C1C-NC	3.02	112.80	109.97
42	F	101	HEM	CMC-C2C-C3C	3.01	130.32	124.68
49	N	623	NEX	C39-C29-C30	-3.01	118.70	122.92
28	Y	604	CLA	C2C-C1C-NC	3.01	112.80	109.97
28	b	602	CLA	CMA-C3A-C4A	3.01	119.87	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S	621	LUT	C15-C14-C13	-3.01	123.01	127.31
28	c	513	CLA	C2C-C1C-NC	3.01	112.79	109.97
28	c	513	CLA	C2D-C1D-ND	3.01	112.32	110.10
46	Y	605	CHL	CMA-C3A-C4A	3.01	119.86	111.77
28	b	611	CLA	CHD-C1D-ND	-3.01	121.69	124.45
28	C	507	CLA	CHD-C1D-ND	-3.01	121.69	124.45
28	B	614	CLA	C1C-C2C-C3C	-3.01	103.80	106.96
28	S	614	CLA	C2C-C1C-NC	3.01	112.79	109.97
28	d	402	CLA	CHD-C1D-ND	-3.01	121.69	124.45
28	G	613	CLA	C2C-C1C-NC	3.00	112.79	109.97
28	C	504	CLA	CHD-C1D-ND	-3.00	121.70	124.45
28	N	610	CLA	C2D-C1D-ND	3.00	112.31	110.10
46	S	601	CHL	CMA-C3A-C4A	3.00	119.83	111.77
28	G	611	CLA	CHD-C1D-ND	-2.99	121.70	124.45
28	N	614	CLA	CMA-C3A-C4A	2.99	119.82	111.77
46	G	609	CHL	C1B-CHB-C4A	-2.99	124.19	130.12
28	B	609	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
46	S	608	CHL	C2C-C3C-C4C	2.99	108.62	106.49
46	N	608	CHL	CMA-C3A-C4A	2.99	119.82	111.77
28	Y	610	CLA	C2D-C1D-ND	2.99	112.31	110.10
46	G	601	CHL	CMA-C3A-C4A	2.99	119.81	111.77
28	S	614	CLA	C1-C2-C3	-2.99	120.87	126.04
28	Y	602	CLA	CHD-C1D-ND	-2.99	121.71	124.45
28	a	406	CLA	CMA-C3A-C4A	2.99	119.81	111.77
28	b	610	CLA	C2D-C1D-ND	2.99	112.31	110.10
28	A	406	CLA	CHD-C1D-ND	-2.99	121.71	124.45
28	B	611	CLA	CHD-C1D-ND	-2.99	121.71	124.45
28	B	614	CLA	C2D-C1D-ND	2.99	112.30	110.10
28	b	609	CLA	C2D-C1D-ND	2.99	112.30	110.10
28	b	617	CLA	C2C-C1C-NC	2.98	112.77	109.97
30	C	517	BCR	C19-C18-C17	2.98	123.52	118.94
28	N	603	CLA	CHD-C1D-ND	-2.98	121.71	124.45
28	C	501	CLA	C2C-C1C-NC	2.98	112.77	109.97
28	G	604	CLA	CHD-C1D-ND	-2.98	121.71	124.45
28	C	513	CLA	C2C-C1C-NC	2.98	112.76	109.97
28	c	502	CLA	C1-C2-C3	-2.98	120.89	126.04
28	S	617	CLA	CMA-C3A-C4A	2.98	119.78	111.77
46	G	606	CHL	CMA-C3A-C4A	2.98	119.78	111.77
28	N	611	CLA	C2D-C1D-ND	2.98	112.30	110.10
28	c	504	CLA	C1C-C2C-C3C	-2.98	103.83	106.96
28	Y	608	CLA	CMA-C3A-C4A	2.98	119.77	111.77
28	c	503	CLA	C2C-C1C-NC	2.98	112.76	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	620	C7Z	C21-C26-C25	-2.98	118.42	122.61
46	Y	607	CHL	C2C-C3C-C4C	2.97	108.61	106.49
28	B	608	CLA	CHD-C1D-ND	-2.97	121.72	124.45
29	A	408	PHO	O1D-CGD-CBD	2.97	129.69	124.74
28	B	609	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
28	b	606	CLA	C1-C2-C3	-2.97	120.91	126.04
28	d	402	CLA	C2C-C1C-NC	2.97	112.75	109.97
41	d	405	PL9	C27-C28-C29	-2.96	120.53	127.66
28	B	611	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
28	B	606	CLA	C1C-C2C-C3C	-2.96	103.85	106.96
28	C	511	CLA	CMA-C3A-C4A	2.96	119.72	111.77
28	G	614	CLA	C2C-C1C-NC	2.96	112.74	109.97
28	S	617	CLA	CHD-C1D-ND	-2.96	121.74	124.45
30	b	618	BCR	C34-C9-C10	-2.95	118.79	122.92
28	S	602	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
28	S	605	CLA	CMA-C3A-C4A	2.95	119.71	111.77
28	a	407	CLA	CHD-C1D-ND	-2.95	121.74	124.45
28	B	612	CLA	C1-C2-C3	-2.95	120.94	126.04
28	Y	603	CLA	C2D-C1D-ND	2.95	112.28	110.10
28	C	507	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
28	B	607	CLA	C2C-C1C-NC	2.95	112.73	109.97
46	Y	607	CHL	CMA-C3A-C4A	2.95	119.70	111.77
28	N	614	CLA	C2D-C1D-ND	2.95	112.28	110.10
28	a	407	CLA	OBD-CAD-C3D	-2.95	121.43	128.52
28	Y	613	CLA	C2C-C1C-NC	2.95	112.73	109.97
28	b	614	CLA	CHD-C1D-ND	-2.94	121.75	124.45
28	Y	613	CLA	CMA-C3A-C4A	2.94	119.68	111.77
28	b	605	CLA	O2A-CGA-CBA	2.94	121.14	111.91
34	B	620	C7Z	C38-C25-C24	2.94	119.80	114.36
28	C	503	CLA	CHD-C1D-ND	-2.94	121.75	124.45
28	B	603	CLA	C2D-C1D-ND	2.94	112.27	110.10
28	S	610	CLA	C2D-C1D-ND	2.93	112.27	110.10
47	S	621	LUT	C35-C15-C14	-2.93	117.47	123.47
28	S	602	CLA	C2D-C1D-ND	2.93	112.26	110.10
28	S	612	CLA	CHD-C1D-ND	-2.93	121.76	124.45
30	b	619	BCR	C33-C5-C6	-2.93	121.24	124.53
28	N	602	CLA	C2D-C1D-ND	2.93	112.26	110.10
28	B	612	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
28	c	508	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
48	N	622	XAT	C7-C8-C9	-2.93	120.99	125.53
28	b	614	CLA	C2D-C1D-ND	2.93	112.26	110.10
28	b	603	CLA	C2D-C1D-ND	2.93	112.26	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	608	CLA	CMA-C3A-C4A	2.92	119.63	111.77
28	b	608	CLA	CHD-C1D-ND	-2.92	121.77	124.45
28	c	501	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
28	C	505	CLA	C1-C2-C3	-2.92	120.99	126.04
28	A	406	CLA	CMA-C3A-C4A	2.92	119.62	111.77
28	a	406	CLA	CHD-C1D-ND	-2.92	121.77	124.45
46	N	606	CHL	CMA-C3A-C4A	2.92	119.62	111.77
28	a	405	CLA	CMB-C2B-C3B	2.92	130.14	124.68
30	D	404	BCR	C36-C18-C17	-2.92	118.83	122.92
46	N	608	CHL	C3C-C4C-NC	-2.92	107.30	110.57
28	B	609	CLA	CMB-C2B-C3B	2.92	130.13	124.68
28	c	502	CLA	C1C-C2C-C3C	-2.91	103.89	106.96
28	b	615	CLA	C2C-C1C-NC	2.91	112.70	109.97
46	N	606	CHL	CHD-C1D-ND	-2.91	121.78	124.45
28	b	605	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
48	N	622	XAT	O4-C5-C4	-2.91	111.19	113.38
28	b	607	CLA	C1-C2-C3	-2.91	121.01	126.04
28	N	610	CLA	C2C-C1C-NC	2.91	112.70	109.97
28	S	602	CLA	O2A-CGA-CBA	2.91	121.04	111.91
28	c	512	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
28	C	503	CLA	C1-C2-C3	-2.91	121.01	126.04
28	C	512	CLA	CMB-C2B-C3B	2.91	130.12	124.68
28	b	610	CLA	C1-C2-C3	-2.91	121.02	126.04
28	b	613	CLA	C2D-C1D-ND	2.91	112.25	110.10
28	Y	611	CLA	CHD-C1D-ND	-2.91	121.78	124.45
28	b	604	CLA	CHD-C1D-ND	-2.91	121.78	124.45
28	b	610	CLA	CMB-C2B-C3B	2.90	130.11	124.68
28	c	505	CLA	C1-O2A-CGA	2.90	124.06	116.44
42	f	101	HEM	C4D-ND-C1D	2.90	108.07	105.07
46	Y	605	CHL	C2C-C3C-C4C	2.90	108.56	106.49
28	N	603	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
28	C	512	CLA	CMA-C3A-C4A	2.90	119.56	111.77
28	S	617	CLA	C2D-C1D-ND	2.90	112.24	110.10
28	B	604	CLA	C1-C2-C3	-2.90	121.03	126.04
28	G	610	CLA	C2D-C1D-ND	2.89	112.24	110.10
46	G	608	CHL	C2C-C3C-C4C	2.89	108.55	106.49
28	S	609	CLA	C2D-C1D-ND	2.89	112.23	110.10
28	A	407	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
28	S	603	CLA	C1-C2-C3	-2.89	121.05	126.04
28	B	610	CLA	O2A-CGA-CBA	2.89	120.97	111.91
47	G	620	LUT	C31-C30-C29	-2.89	123.19	127.31
34	B	620	C7Z	C11-C12-C13	-2.89	118.31	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	612	CLA	CMB-C2B-C3B	2.88	130.07	124.68
28	b	614	CLA	C1C-C2C-C3C	-2.88	103.92	106.96
28	G	603	CLA	CMA-C3A-C4A	2.88	119.52	111.77
28	a	406	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
28	B	616	CLA	C2D-C1D-ND	2.88	112.23	110.10
28	a	410	CLA	CHD-C1D-ND	-2.88	121.81	124.45
30	C	516	BCR	C34-C9-C10	-2.88	118.89	122.92
28	c	508	CLA	CMA-C3A-C4A	2.88	119.51	111.77
28	A	407	CLA	CHD-C1D-ND	-2.88	121.81	124.45
46	Y	607	CHL	C3C-C4C-NC	-2.88	107.34	110.57
28	B	609	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
28	c	504	CLA	CHD-C1D-ND	-2.88	121.81	124.45
47	G	620	LUT	C11-C10-C9	-2.87	123.21	127.31
30	C	514	BCR	C38-C26-C25	-2.87	121.30	124.53
28	S	611	CLA	CMA-C3A-C4A	2.87	119.50	111.77
28	c	512	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
28	G	613	CLA	C2D-C1D-ND	2.87	112.22	110.10
46	S	608	CHL	C3C-C4C-NC	-2.87	107.35	110.57
30	c	517	BCR	C36-C18-C17	-2.87	118.90	122.92
32	d	411	LMG	O8-C28-C29	2.87	120.91	111.91
28	C	501	CLA	C2D-C1D-ND	2.87	112.22	110.10
28	B	603	CLA	CMA-C3A-C4A	2.87	119.48	111.77
28	Y	610	CLA	C2C-C1C-NC	2.87	112.66	109.97
28	Y	603	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
28	G	602	CLA	C2D-C1D-ND	2.87	112.22	110.10
34	B	620	C7Z	C22-C23-C24	2.87	114.23	110.30
28	N	604	CLA	CHD-C1D-ND	-2.87	121.82	124.45
28	c	501	CLA	C2C-C1C-NC	2.87	112.66	109.97
28	Y	612	CLA	C1C-C2C-C3C	-2.86	103.94	106.96
38	l	101	LHG	O8-C23-C24	2.86	120.89	111.91
28	a	405	CLA	C1D-ND-C4D	-2.86	104.30	106.33
28	B	615	CLA	CMB-C2B-C3B	2.86	130.03	124.68
28	A	410	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
28	b	611	CLA	C1D-ND-C4D	-2.86	104.30	106.33
28	S	613	CLA	C2D-C1D-ND	2.86	112.21	110.10
28	a	406	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
28	c	506	CLA	CHD-C1D-ND	-2.86	121.83	124.45
38	d	410	LHG	O8-C23-C24	2.86	120.87	111.91
28	b	608	CLA	C1-C2-C3	-2.86	121.10	126.04
28	B	602	CLA	CHD-C1D-ND	-2.86	121.83	124.45
38	D	410	LHG	O8-C23-C24	2.85	120.87	111.91
28	B	610	CLA	C2D-C1D-ND	2.85	112.21	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	507	CLA	CMA-C3A-C4A	2.85	119.44	111.77
28	B	616	CLA	CHD-C1D-ND	-2.85	121.83	124.45
46	Y	607	CHL	CHB-C4A-NA	2.85	128.46	124.51
28	B	606	CLA	C2D-C1D-ND	2.85	112.20	110.10
46	N	609	CHL	C3C-C4C-NC	-2.85	107.38	110.57
47	Y	620	LUT	C18-C5-C6	-2.85	121.33	124.53
28	A	407	CLA	C2D-C1D-ND	2.85	112.20	110.10
28	b	616	CLA	C2D-C1D-ND	2.85	112.20	110.10
28	C	511	CLA	C1-C2-C3	-2.85	121.12	126.04
28	G	612	CLA	CHD-C1D-ND	-2.85	121.84	124.45
28	G	613	CLA	CHD-C1D-ND	-2.85	121.84	124.45
30	A	411	BCR	C33-C5-C4	2.85	119.08	113.62
28	N	611	CLA	CHD-C1D-ND	-2.84	121.84	124.45
28	c	512	CLA	C2D-C1D-ND	2.84	112.20	110.10
28	A	410	CLA	CMA-C3A-C4A	2.84	119.41	111.77
28	S	603	CLA	C2D-C1D-ND	2.84	112.20	110.10
46	N	605	CHL	CMA-C3A-C4A	2.84	119.41	111.77
28	C	513	CLA	C1-C2-C3	-2.84	121.13	126.04
28	A	406	CLA	CMB-C2B-C3B	2.84	129.99	124.68
28	N	604	CLA	C2D-C1D-ND	2.84	112.20	110.10
46	G	609	CHL	C1-O2A-CGA	2.84	123.89	116.44
28	B	616	CLA	C1-C2-C3	-2.84	121.14	126.04
47	Y	620	LUT	C38-C25-C24	-2.84	117.49	123.56
28	c	505	CLA	CMA-C3A-C4A	2.84	119.39	111.77
28	a	407	CLA	C2C-C1C-NC	2.83	112.63	109.97
48	G	622	XAT	C26-C27-C28	-2.83	120.00	125.99
28	d	403	CLA	C2C-C1C-NC	2.83	112.63	109.97
49	G	623	NEX	C38-C25-C26	-2.83	117.51	122.26
29	A	408	PHO	CMB-C2B-C3B	2.83	129.98	124.68
28	C	502	CLA	CHD-C1D-ND	-2.83	121.85	124.45
29	a	408	PHO	O1D-CGD-CBD	2.83	129.46	124.74
30	c	515	BCR	C23-C24-C25	-2.83	119.25	127.20
46	Y	607	CHL	C4A-NA-C1A	2.83	107.98	106.71
28	G	604	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
43	h	101	RRX	C33-C5-C4	2.83	119.05	113.62
32	C	523	LMG	O8-C28-C29	2.83	120.78	111.91
28	c	502	CLA	C2D-C1D-ND	2.83	112.19	110.10
28	N	613	CLA	C2D-C1D-ND	2.82	112.19	110.10
28	B	612	CLA	CHD-C1D-ND	-2.82	121.86	124.45
28	G	610	CLA	C2C-C1C-NC	2.82	112.62	109.97
28	S	605	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
28	S	611	CLA	C1C-C2C-C3C	-2.82	103.99	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	409	PHO	O1D-CGD-CBD	2.82	129.44	124.74
28	c	507	CLA	CHD-C1D-ND	-2.82	121.86	124.45
46	N	605	CHL	C1-C2-C3	-2.82	121.17	126.04
28	S	604	CLA	C1C-C2C-C3C	-2.82	104.00	106.96
28	G	603	CLA	C2D-C1D-ND	2.81	112.18	110.10
46	G	606	CHL	CHB-C4A-NA	2.81	128.40	124.51
28	b	610	CLA	C2C-C1C-NC	2.81	112.61	109.97
28	A	410	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
28	Y	602	CLA	C1-C2-C3	-2.81	121.19	126.04
28	B	617	CLA	C1-C2-C3	-2.81	121.19	126.04
28	b	613	CLA	C2C-C1C-NC	2.81	112.60	109.97
46	G	607	CHL	C1-O2A-CGA	2.81	123.81	116.44
28	B	610	CLA	CHD-C1D-ND	-2.81	121.88	124.45
32	W	201	LMG	O8-C28-C29	2.81	120.71	111.91
28	B	608	CLA	CMA-C3A-C4A	2.80	119.31	111.77
28	c	513	CLA	CAA-C2A-C3A	-2.80	105.10	112.78
46	N	606	CHL	C3C-C4C-NC	-2.80	107.43	110.57
28	Y	614	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
28	B	604	CLA	CHD-C1D-ND	-2.80	121.88	124.45
28	Y	612	CLA	CHD-C1D-ND	-2.80	121.88	124.45
49	N	623	NEX	C19-C9-C10	-2.80	119.00	122.92
41	d	405	PL9	C40-C39-C41	2.80	119.98	115.27
28	b	615	CLA	CMB-C2B-C3B	2.80	129.92	124.68
32	c	521	LMG	O8-C28-C29	2.80	120.69	111.91
28	N	612	CLA	CHD-C1D-ND	-2.80	121.88	124.45
29	a	408	PHO	CMB-C2B-C3B	2.80	129.91	124.68
47	Y	620	LUT	C11-C10-C9	-2.80	123.32	127.31
28	N	614	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
28	N	612	CLA	C2D-C1D-ND	2.80	112.17	110.10
28	a	407	CLA	CHA-C4D-ND	2.79	138.34	132.50
35	C	519	DGD	O1G-C1A-C2A	2.79	120.68	111.91
30	C	515	BCR	C34-C9-C10	-2.79	119.01	122.92
28	b	612	CLA	CHD-C1D-ND	-2.79	121.89	124.45
47	S	620	LUT	C22-C23-C24	-2.79	108.56	111.74
28	Y	613	CLA	C2D-C1D-ND	2.79	112.16	110.10
28	S	613	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
28	c	505	CLA	CHD-C1D-ND	-2.79	121.89	124.45
47	N	620	LUT	C18-C5-C6	-2.78	121.40	124.53
47	N	620	LUT	C38-C25-C24	-2.78	117.60	123.56
28	N	603	CLA	C2D-C1D-ND	2.78	112.16	110.10
28	G	602	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
28	B	612	CLA	C2D-C1D-ND	2.78	112.16	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Y	602	CLA	CMA-C3A-C4A	2.78	119.25	111.77
28	A	410	CLA	C1-C2-C3	-2.78	121.23	126.04
28	S	614	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
28	B	611	CLA	C2D-C1D-ND	2.78	112.15	110.10
28	C	512	CLA	O2A-CGA-CBA	2.78	120.63	111.91
28	S	611	CLA	C2D-C1D-ND	2.78	112.15	110.10
28	c	509	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
28	c	512	CLA	CMA-C3A-C4A	2.78	119.23	111.77
46	G	607	CHL	CHB-C4A-NA	2.78	128.35	124.51
30	c	516	BCR	C33-C5-C4	2.78	118.95	113.62
28	G	614	CLA	CMA-C3A-C4A	2.77	119.23	111.77
28	B	605	CLA	O2A-CGA-CBA	2.77	120.61	111.91
46	G	609	CHL	C4D-CHA-C1A	2.77	124.62	121.25
28	c	502	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
41	d	405	PL9	C7-C8-C9	-2.77	122.18	126.79
28	b	604	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
28	Y	610	CLA	O2A-CGA-CBA	2.77	120.59	111.91
38	D	409	LHG	O8-C23-C24	2.77	120.58	111.91
28	B	603	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
29	a	409	PHO	O2D-CGD-O1D	-2.76	118.44	123.84
28	D	402	CLA	C1D-ND-C4D	-2.76	104.37	106.33
30	B	618	BCR	C23-C24-C25	-2.76	119.45	127.20
28	C	513	CLA	CMA-C3A-C4A	2.76	119.19	111.77
28	Y	602	CLA	C2D-C1D-ND	2.76	112.14	110.10
28	b	612	CLA	C2D-C1D-ND	2.76	112.14	110.10
28	b	603	CLA	CMA-C3A-C4A	2.75	119.18	111.77
46	N	608	CHL	C2C-C3C-C4C	2.75	108.45	106.49
28	C	504	CLA	C2C-C1C-NC	2.75	112.55	109.97
35	c	520	DGD	O1G-C1A-C2A	2.75	120.55	111.91
28	Y	604	CLA	C1-C2-C3	-2.75	121.28	126.04
28	D	403	CLA	O2A-CGA-CBA	2.75	120.54	111.91
46	N	609	CHL	C1-O2A-CGA	2.75	123.66	116.44
35	C	518	DGD	O1G-C1A-C2A	2.75	120.54	111.91
28	c	509	CLA	CMA-C3A-C4A	2.75	119.16	111.77
28	b	609	CLA	CHD-C1D-ND	-2.75	121.93	124.45
30	C	514	BCR	C23-C24-C25	-2.75	119.48	127.20
28	N	602	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
28	A	410	CLA	CAA-C2A-C3A	-2.75	105.26	112.78
28	G	614	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
28	N	613	CLA	CHD-C1D-ND	-2.74	121.93	124.45
50	S	625	LPX	O3-P1-O4	2.74	125.80	112.24
49	Y	623	NEX	C16-C1-C6	-2.74	108.02	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	603	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
28	C	502	CLA	C2D-C1D-ND	2.74	112.12	110.10
28	b	612	CLA	CMA-C3A-C4A	2.74	119.14	111.77
28	C	505	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
28	b	617	CLA	C2D-C1D-ND	2.74	112.12	110.10
28	G	610	CLA	O2A-CGA-CBA	2.74	120.50	111.91
28	D	403	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
51	Y	626	PTY	O4-C30-C31	2.74	120.50	111.91
28	b	605	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
28	S	603	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
28	G	604	CLA	CMA-C3A-C4A	2.73	119.12	111.77
28	C	512	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
28	c	512	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
48	Y	622	XAT	C38-C25-C26	-2.73	117.69	122.26
49	S	623	NEX	C38-C25-C26	-2.73	117.69	122.26
28	Y	613	CLA	O2A-CGA-CBA	2.73	120.47	111.91
28	Y	608	CLA	C2D-C1D-ND	2.73	112.11	110.10
28	d	402	CLA	C2D-C1D-ND	2.73	112.11	110.10
36	t	101	3PH	O31-C31-C32	2.72	120.46	111.91
28	c	501	CLA	C2D-C1D-ND	2.72	112.11	110.10
38	C	525	LHG	O8-C23-C24	2.72	120.46	111.91
34	B	620	C7Z	C28-C27-C26	-2.72	119.56	127.20
46	Y	601	CHL	CHB-C4A-NA	2.72	128.28	124.51
28	B	602	CLA	CMA-C3A-C4A	2.72	119.09	111.77
46	N	607	CHL	CMA-C3A-C4A	2.72	119.09	111.77
43	h	101	RRX	C2-C1-C6	2.72	114.67	110.48
38	d	409	LHG	O8-C23-C24	2.72	120.44	111.91
28	S	617	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
28	B	605	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
38	L	101	LHG	O8-C23-C24	2.72	120.43	111.91
28	N	613	CLA	C1-C2-C3	-2.72	121.34	126.04
28	G	611	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
28	Y	614	CLA	C2D-C1D-ND	2.72	112.11	110.10
28	S	611	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
28	N	602	CLA	CMA-C3A-C4A	2.71	119.07	111.77
28	G	614	CLA	C2D-C1D-ND	2.71	112.10	110.10
46	G	608	CHL	C3C-C4C-NC	-2.71	107.53	110.57
43	h	101	RRX	C30-C25-C26	-2.71	118.80	122.61
28	a	410	CLA	O2A-CGA-CBA	2.71	120.40	111.91
28	N	604	CLA	OBD-CAD-C3D	-2.71	122.01	128.52
34	B	620	C7Z	C18-C5-C4	2.70	119.36	114.36
28	S	602	CLA	C2C-C1C-NC	2.70	112.50	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	411	BCR	C36-C18-C17	-2.70	119.14	122.92
30	C	515	BCR	C23-C24-C25	-2.70	119.62	127.20
49	Y	623	NEX	C38-C25-C26	-2.70	117.74	122.26
28	D	403	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
28	b	614	CLA	CMB-C2B-C3B	2.70	129.72	124.68
30	C	516	BCR	C27-C26-C25	-2.70	118.82	122.73
35	C	520	DGD	O1G-C1A-C2A	2.69	120.36	111.91
28	B	602	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
28	D	402	CLA	CHA-C4D-ND	2.69	138.13	132.50
28	C	512	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
28	S	611	CLA	CHD-C1D-ND	-2.69	121.98	124.45
42	F	101	HEM	C4D-ND-C1D	2.69	107.85	105.07
46	Y	601	CHL	C1-C2-C3	-2.69	121.40	126.04
28	B	617	CLA	C2D-C1D-ND	2.69	112.08	110.10
28	b	604	CLA	CMA-C3A-C4A	2.69	118.99	111.77
32	C	521	LMG	O8-C28-C29	2.69	120.34	111.91
28	c	511	CLA	C2D-C1D-ND	2.69	112.08	110.10
28	C	510	CLA	CMD-C2D-C3D	-2.68	121.44	127.61
28	b	609	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
28	b	613	CLA	C1-C2-C3	-2.68	121.40	126.04
28	c	512	CLA	C1-C2-C3	-2.68	121.40	126.04
45	K	101	4RF	O18-C16-C15	2.68	120.32	111.91
28	A	410	CLA	C2D-C1D-ND	2.68	112.08	110.10
47	N	620	LUT	C7-C8-C9	-2.68	122.19	126.23
28	b	602	CLA	C1-C2-C3	-2.68	121.41	126.04
35	c	519	DGD	O1G-C1A-C2A	2.68	120.31	111.91
28	B	615	CLA	CMD-C2D-C3D	-2.68	121.45	127.61
28	B	607	CLA	O2A-CGA-CBA	2.68	120.31	111.91
28	B	608	CLA	CMD-C2D-C3D	-2.68	121.45	127.61
30	d	404	BCR	C38-C26-C25	-2.68	121.52	124.53
28	b	609	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
30	D	404	BCR	C38-C26-C25	-2.68	121.52	124.53
28	B	605	CLA	CHD-C1D-ND	-2.68	122.00	124.45
28	B	607	CLA	C1-C2-C3	-2.68	121.42	126.04
28	c	513	CLA	CMA-C3A-C4A	2.68	118.96	111.77
28	B	613	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
28	G	604	CLA	C2D-C1D-ND	2.67	112.08	110.10
28	Y	604	CLA	C2D-C1D-ND	2.67	112.08	110.10
28	C	509	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
45	I	102	4RF	O40-C41-C43	2.67	120.30	111.91
28	B	608	CLA	C1-C2-C3	-2.67	121.42	126.04
28	d	403	CLA	C2D-C1D-ND	2.67	112.07	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S	608	CHL	C1-O2A-CGA	2.67	123.45	116.44
32	A	413	LMG	C8-O7-C10	-2.67	111.21	117.79
28	b	605	CLA	CHD-C1D-ND	-2.67	122.00	124.45
28	N	612	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
28	b	606	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
28	c	512	CLA	O2A-CGA-CBA	2.67	120.28	111.91
46	Y	601	CHL	C3C-C4C-NC	-2.67	107.58	110.57
47	G	620	LUT	C38-C25-C24	-2.66	117.86	123.56
28	C	508	CLA	CMA-C3A-C4A	2.66	118.93	111.77
46	N	601	CHL	C1-C2-C3	-2.66	121.44	126.04
30	a	411	BCR	C38-C26-C27	2.66	118.73	113.62
28	S	612	CLA	CMB-C2B-C1B	-2.66	124.38	128.46
28	C	505	CLA	CHA-C4D-ND	2.66	138.06	132.50
28	C	502	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
37	J	101	DGA	OG1-CA1-CA2	2.66	120.24	111.91
28	B	615	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
28	C	503	CLA	C2D-C1D-ND	2.66	112.06	110.10
28	C	504	CLA	CMA-C3A-C4A	2.66	118.91	111.77
28	N	611	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
30	c	516	BCR	C34-C9-C10	-2.65	119.20	122.92
28	Y	608	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
28	b	608	CLA	C2D-C1D-ND	2.65	112.06	110.10
28	N	602	CLA	O2A-CGA-CBA	2.65	120.23	111.91
37	C	524	DGA	OG1-CA1-CA2	2.65	120.23	111.91
28	b	606	CLA	CMD-C2D-C3D	-2.65	121.52	127.61
42	F	101	HEM	C4B-CHC-C1C	2.65	126.06	122.56
30	c	517	BCR	C33-C5-C6	-2.65	121.55	124.53
28	B	605	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
38	D	410	LHG	C5-O7-C7	-2.65	111.27	117.79
30	b	618	BCR	C38-C26-C27	2.65	118.70	113.62
28	Y	602	CLA	O2A-CGA-CBA	2.65	120.22	111.91
46	Y	606	CHL	C1-C2-C3	-2.65	121.46	126.04
36	T	101	3PH	O31-C31-C32	2.65	120.22	111.91
28	c	505	CLA	O2A-CGA-CBA	2.65	120.21	111.91
29	A	409	PHO	O2D-CGD-O1D	-2.64	118.67	123.84
30	C	517	BCR	C23-C24-C25	-2.64	119.78	127.20
46	Y	609	CHL	C1-O2A-CGA	2.64	123.38	116.44
28	Y	613	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
28	d	403	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
28	b	602	CLA	C2D-C1D-ND	2.64	112.05	110.10
28	c	513	CLA	CMB-C2B-C3B	2.64	129.62	124.68
28	B	612	CLA	C2C-C1C-NC	2.64	112.45	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	S	624	LHG	O8-C23-C24	2.64	120.20	111.91
28	Y	603	CLA	CMA-C3A-C4A	2.64	118.87	111.77
28	G	612	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
28	G	612	CLA	C2D-C1D-ND	2.64	112.05	110.10
28	Y	611	CLA	C2D-C1D-ND	2.64	112.05	110.10
47	Y	620	LUT	C10-C11-C12	-2.64	114.98	123.22
28	C	513	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
46	G	606	CHL	C1-O2A-CGA	2.64	123.36	116.44
34	b	620	C7Z	C28-C27-C26	-2.64	119.80	127.20
28	B	615	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
28	C	506	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
46	G	605	CHL	CHB-C4A-NA	2.63	128.15	124.51
47	G	620	LUT	C18-C5-C6	-2.63	121.57	124.53
28	Y	602	CLA	C2C-C1C-NC	2.63	112.44	109.97
28	S	605	CLA	O2A-CGA-CBA	2.63	120.17	111.91
28	C	511	CLA	C2D-C1D-ND	2.63	112.04	110.10
46	N	608	CHL	C1B-CHB-C4A	-2.63	124.91	130.12
28	c	507	CLA	O2A-CGA-CBA	2.63	120.16	111.91
28	A	410	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
35	b	623	DGD	O1G-C1A-C2A	2.63	120.16	111.91
28	S	604	CLA	O2A-CGA-CBA	2.63	120.16	111.91
30	C	514	BCR	C40-C30-C25	-2.63	106.04	110.30
46	N	609	CHL	C1B-CHB-C4A	-2.63	124.91	130.12
28	S	605	CLA	CHA-C4D-ND	2.63	137.99	132.50
28	c	510	CLA	C1D-ND-C4D	-2.63	104.47	106.33
28	b	602	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
28	b	616	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
47	Y	620	LUT	C31-C30-C29	-2.63	123.56	127.31
28	S	605	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
28	c	505	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
28	S	602	CLA	O1D-CGD-CBD	-2.62	119.12	124.48
28	b	615	CLA	CMD-C2D-C3D	-2.62	121.58	127.61
28	c	506	CLA	CMA-C3A-C4A	2.62	118.82	111.77
30	C	514	BCR	C38-C26-C27	2.62	118.66	113.62
28	C	507	CLA	C1-O2A-CGA	2.62	123.33	116.44
28	B	613	CLA	CHA-C4D-ND	2.62	137.99	132.50
32	a	413	LMG	O8-C28-C29	2.62	120.14	111.91
30	B	618	BCR	C4-C5-C6	-2.62	118.93	122.73
28	A	405	CLA	C2C-C1C-NC	2.62	112.43	109.97
28	N	602	CLA	C2C-C1C-NC	2.62	112.43	109.97
28	b	615	CLA	C2D-C1D-ND	2.62	112.03	110.10
32	c	523	LMG	O8-C28-C29	2.62	120.13	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	H	101	RRX	C30-C25-C26	-2.62	118.92	122.61
28	B	606	CLA	C1-O2A-CGA	2.62	123.31	116.44
28	Y	612	CLA	O2A-CGA-CBA	2.62	120.12	111.91
28	C	511	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
28	a	410	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
28	G	602	CLA	C1-C2-C3	-2.62	121.52	126.04
28	B	606	CLA	CMD-C2D-C3D	-2.62	121.59	127.61
41	d	405	PL9	C22-C23-C24	-2.62	121.36	127.66
47	N	621	LUT	C38-C25-C24	-2.62	117.96	123.56
30	B	618	BCR	C34-C9-C10	-2.62	119.26	122.92
28	B	608	CLA	CHA-C4D-ND	2.61	137.97	132.50
28	c	505	CLA	O1D-CGD-CBD	-2.61	119.14	124.48
28	B	609	CLA	CMA-C3A-C4A	2.61	118.79	111.77
28	c	501	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
47	Y	621	LUT	C38-C25-C24	-2.61	117.97	123.56
28	B	604	CLA	O2A-CGA-CBA	2.61	120.10	111.91
43	h	101	RRX	C7-C6-C5	-2.61	115.14	121.46
38	D	408	LHG	O8-C23-C24	2.61	120.10	111.91
28	b	610	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
46	N	609	CHL	C4A-NA-C1A	2.61	107.88	106.71
46	Y	605	CHL	CHB-C4A-NA	2.61	128.12	124.51
28	B	604	CLA	CHA-C4D-ND	2.61	137.95	132.50
28	S	603	CLA	CHA-C4D-ND	2.61	137.95	132.50
30	C	516	BCR	C28-C27-C26	-2.61	109.42	114.08
28	B	604	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
28	N	611	CLA	CMA-C3A-C4A	2.60	118.77	111.77
28	b	611	CLA	CMA-C3A-C4A	2.60	118.77	111.77
49	S	623	NEX	C39-C29-C30	-2.60	119.28	122.92
30	B	618	BCR	C1-C6-C7	2.60	123.14	115.78
36	b	624	3PH	O31-C31-C32	2.60	120.08	111.91
28	B	615	CLA	CHA-C4D-ND	2.60	137.94	132.50
28	S	617	CLA	O2A-CGA-CBA	2.60	120.08	111.91
43	H	101	RRX	C36-C18-C19	2.60	122.18	118.08
47	G	621	LUT	C35-C15-C14	-2.60	118.14	123.47
28	B	613	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
28	C	513	CLA	CBA-CAA-C2A	2.60	121.54	113.86
46	G	605	CHL	C4A-NA-C1A	2.60	107.88	106.71
47	Y	621	LUT	C31-C30-C29	-2.60	123.60	127.31
28	C	511	CLA	O2A-CGA-CBA	2.60	120.06	111.91
28	S	612	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
28	C	509	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
35	c	518	DGD	O1G-C1A-C2A	2.60	120.06	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	510	CLA	C2D-C1D-ND	2.60	112.02	110.10
28	C	506	CLA	C1-C2-C3	-2.59	121.56	126.04
28	S	602	CLA	CMA-C3A-C4A	2.59	118.74	111.77
28	B	613	CLA	C1-C2-C3	-2.59	121.56	126.04
28	N	604	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
42	f	101	HEM	C4B-CHC-C1C	2.59	125.98	122.56
28	G	602	CLA	CHD-C1D-ND	-2.59	122.07	124.45
46	S	608	CHL	CHB-C4A-NA	2.59	128.09	124.51
37	j	101	DGA	OG1-CA1-CA2	2.59	120.04	111.91
28	C	501	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
28	B	609	CLA	C2D-C1D-ND	2.59	112.01	110.10
36	S	626	3PH	O31-C31-C32	2.59	120.03	111.91
28	B	611	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
38	Y	624	LHG	C6-C5-C4	-2.59	105.67	111.79
28	G	604	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
28	N	604	CLA	CHA-C4D-ND	2.59	137.91	132.50
30	C	516	BCR	C33-C5-C4	2.58	118.58	113.62
28	S	605	CLA	CHD-C1D-ND	-2.58	122.08	124.45
28	b	605	CLA	CHA-C4D-ND	2.58	137.90	132.50
28	N	610	CLA	C1-C2-C3	-2.58	121.58	126.04
28	D	403	CLA	CMA-C3A-C4A	2.58	118.72	111.77
28	A	405	CLA	CHA-C4D-ND	2.58	137.90	132.50
28	a	410	CLA	CMB-C2B-C1B	-2.58	124.50	128.46
28	S	604	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
28	C	505	CLA	CMB-C2B-C3B	2.58	129.51	124.68
28	B	617	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
28	C	501	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
28	c	501	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
28	d	402	CLA	C1-C2-C3	-2.58	121.58	126.04
28	Y	611	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
28	C	508	CLA	C2D-C1D-ND	2.58	112.00	110.10
29	A	409	PHO	O1D-CGD-CBD	2.58	129.03	124.74
28	c	511	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
28	c	508	CLA	C1D-ND-C4D	-2.57	104.51	106.33
28	c	503	CLA	CMB-C2B-C3B	2.57	129.49	124.68
28	S	611	CLA	CHA-C4D-ND	2.57	137.88	132.50
28	b	608	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
30	b	618	BCR	C28-C27-C26	-2.57	109.49	114.08
28	G	604	CLA	CHA-C4D-ND	2.57	137.88	132.50
45	i	101	4RF	O40-C41-C43	2.57	119.97	111.91
30	b	618	BCR	C1-C6-C5	-2.57	119.00	122.61
28	B	607	CLA	CMB-C2B-C3B	2.57	129.48	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	C	527	LMK	O3-C4-C3	-2.57	114.18	122.98
28	B	602	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
28	B	609	CLA	CHA-C4D-ND	2.57	137.87	132.50
28	c	502	CLA	CMB-C2B-C3B	2.56	129.47	124.68
28	a	407	CLA	CMD-C2D-C3D	-2.56	121.72	127.61
28	a	406	CLA	CHA-C4D-ND	2.56	137.85	132.50
28	b	607	CLA	C2D-C1D-ND	2.56	111.99	110.10
28	G	611	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
41	D	405	PL9	C7-C8-C9	-2.56	122.53	126.79
28	C	506	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
28	C	508	CLA	C2C-C1C-NC	2.56	112.37	109.97
28	Y	611	CLA	C1-C2-C3	-2.56	121.62	126.04
47	N	621	LUT	C35-C15-C14	-2.56	118.24	123.47
28	N	603	CLA	CMA-C3A-C4A	2.56	118.64	111.77
36	B	624	3PH	O31-C31-C32	2.56	119.93	111.91
28	N	604	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
30	b	619	BCR	C4-C5-C6	-2.55	119.02	122.73
28	c	513	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
28	C	510	CLA	CHA-C4D-ND	2.55	137.83	132.50
28	N	611	CLA	CHA-C4D-ND	2.55	137.83	132.50
28	S	603	CLA	CHD-C1D-ND	-2.55	122.11	124.45
28	b	615	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
48	G	622	XAT	C6-C7-C8	-2.55	120.60	125.99
46	Y	609	CHL	C1B-CHB-C4A	-2.55	125.07	130.12
49	Y	623	NEX	C1-C2-C3	2.55	119.39	113.64
28	C	507	CLA	C2D-C1D-ND	2.54	111.98	110.10
28	S	604	CLA	C1-O2A-CGA	2.54	123.12	116.44
28	c	504	CLA	C2D-C1D-ND	2.54	111.98	110.10
28	b	613	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
46	S	601	CHL	CHB-C4A-NA	2.54	128.03	124.51
32	w	201	LMG	O8-C28-C29	2.54	119.88	111.91
28	c	505	CLA	C2D-C1D-ND	2.54	111.98	110.10
28	G	611	CLA	C1-C2-C3	-2.54	121.65	126.04
47	S	620	LUT	C38-C25-C24	-2.54	118.13	123.56
28	c	508	CLA	C2C-C1C-NC	2.54	112.35	109.97
28	B	608	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
28	Y	604	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
30	d	404	BCR	C15-C14-C13	-2.54	123.69	127.31
28	B	603	CLA	C1-O2A-CGA	2.54	123.10	116.44
28	b	613	CLA	CHD-C1D-ND	-2.54	122.12	124.45
28	C	510	CLA	C1D-ND-C4D	-2.54	104.53	106.33
28	a	410	CLA	C2D-C1D-ND	2.53	111.97	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	503	CLA	CHA-C4D-ND	2.53	137.80	132.50
28	S	602	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
28	N	603	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
28	B	603	CLA	O2A-CGA-CBA	2.53	119.86	111.91
32	D	411	LMG	O8-C28-C29	2.53	119.86	111.91
28	B	604	CLA	CMA-C3A-C4A	2.53	118.58	111.77
28	b	604	CLA	O2A-CGA-CBA	2.53	119.85	111.91
28	b	615	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
30	D	404	BCR	C19-C18-C17	2.53	122.83	118.94
28	G	613	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
28	Y	611	CLA	CHA-C4D-ND	2.53	137.79	132.50
28	c	512	CLA	CHA-C4D-ND	2.53	137.79	132.50
28	C	507	CLA	CHA-C4D-ND	2.53	137.79	132.50
28	C	505	CLA	O2A-CGA-CBA	2.53	119.84	111.91
28	c	506	CLA	C2D-C1D-ND	2.53	111.97	110.10
28	B	607	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
46	N	608	CHL	C1-O2A-CGA	2.53	123.07	116.44
38	N	624	LHG	O8-C23-C24	2.53	119.83	111.91
28	Y	611	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
28	G	610	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
43	H	101	RRX	C11-C12-C13	-2.52	119.33	126.42
46	N	606	CHL	CHB-C4A-NA	2.52	128.00	124.51
28	B	607	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
38	c	525	LHG	O8-C23-C24	2.52	119.82	111.91
28	D	402	CLA	C2C-C1C-NC	2.52	112.33	109.97
28	C	511	CLA	CHA-C4D-ND	2.52	137.77	132.50
28	N	612	CLA	CHA-C4D-ND	2.52	137.77	132.50
46	N	609	CHL	C4D-CHA-C1A	2.52	124.31	121.25
30	A	411	BCR	C38-C26-C25	-2.52	121.70	124.53
47	S	620	LUT	C11-C10-C9	-2.52	123.72	127.31
32	B	622	LMG	O8-C28-C29	2.52	119.81	111.91
45	i	101	4RF	O18-C16-C15	2.52	119.81	111.91
28	b	606	CLA	C1D-ND-C4D	-2.52	104.55	106.33
28	S	610	CLA	C1-C2-C3	-2.52	121.69	126.04
28	b	607	CLA	CHA-C4D-ND	2.52	137.76	132.50
28	B	616	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
28	N	613	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
28	B	607	CLA	CHA-C4D-ND	2.51	137.76	132.50
28	N	603	CLA	CHA-C4D-ND	2.51	137.76	132.50
28	C	507	CLA	O2A-CGA-CBA	2.51	119.80	111.91
28	c	512	CLA	CHD-C1D-ND	-2.51	122.14	124.45
28	B	605	CLA	CHA-C4D-ND	2.51	137.76	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	612	CLA	CHA-C4D-ND	2.51	137.75	132.50
28	C	512	CLA	CMB-C2B-C1B	-2.51	124.60	128.46
32	b	622	LMG	O8-C28-C29	2.51	119.79	111.91
28	C	506	CLA	CMA-C3A-C4A	2.51	118.52	111.77
28	d	403	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
28	d	402	CLA	O2A-CGA-CBA	2.51	119.79	111.91
28	c	507	CLA	CHA-C4D-ND	2.51	137.75	132.50
28	C	504	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
28	C	505	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
46	N	601	CHL	CHB-C4A-NA	2.51	127.98	124.51
28	A	406	CLA	CMB-C2B-C1B	-2.51	124.61	128.46
28	Y	610	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
28	B	615	CLA	OBD-CAD-C3D	-2.51	122.48	128.52
46	N	605	CHL	CHB-C4A-NA	2.51	127.98	124.51
28	Y	608	CLA	CHA-C4D-ND	2.51	137.74	132.50
29	a	409	PHO	CMC-C2C-C3C	2.51	129.67	124.94
28	B	608	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
45	K	101	4RF	O40-C41-C43	2.51	119.77	111.91
28	N	611	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
28	c	510	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
28	a	410	CLA	CHA-C4D-ND	2.50	137.74	132.50
28	b	604	CLA	CHA-C4D-ND	2.50	137.74	132.50
38	G	624	LHG	O8-C23-C24	2.50	119.76	111.91
45	I	102	4RF	O18-C16-C15	2.50	119.76	111.91
30	b	618	BCR	C36-C18-C17	-2.50	119.42	122.92
28	b	610	CLA	CHA-C4D-ND	2.50	137.73	132.50
28	b	617	CLA	CMA-C3A-C4A	2.50	118.50	111.77
28	b	615	CLA	CHA-C4D-ND	2.50	137.73	132.50
28	d	402	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
43	H	101	RRX	C8-C7-C6	-2.50	120.18	127.20
28	S	609	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
28	c	513	CLA	CBA-CAA-C2A	2.50	121.24	113.86
28	b	616	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
28	S	603	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
28	S	614	CLA	CHA-C4D-ND	2.50	137.72	132.50
37	c	524	DGA	OG1-CA1-CA2	2.50	119.74	111.91
28	Y	602	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
47	Y	621	LUT	C3-C4-C5	-2.50	106.88	111.85
46	Y	607	CHL	C1-O2A-CGA	2.50	122.99	116.44
30	a	411	BCR	C23-C24-C25	-2.50	120.19	127.20
28	B	611	CLA	CMA-C3A-C4A	2.49	118.48	111.77
30	c	517	BCR	C8-C9-C10	2.49	122.77	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Y	613	CLA	CMB-C2B-C3B	2.49	129.34	124.68
28	b	609	CLA	CHA-C4D-ND	2.49	137.72	132.50
28	G	614	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
28	c	507	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
30	c	514	BCR	C36-C18-C17	-2.49	119.43	122.92
28	b	614	CLA	CHA-C4D-ND	2.49	137.71	132.50
30	c	517	BCR	C15-C14-C13	-2.49	123.75	127.31
30	c	516	BCR	C37-C22-C23	2.49	122.00	118.08
28	a	407	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
28	S	610	CLA	C2C-C1C-NC	2.49	112.31	109.97
28	C	506	CLA	CHA-C4D-ND	2.49	137.71	132.50
46	G	609	CHL	CHC-C1C-NC	2.49	127.98	124.20
49	S	623	NEX	C19-C9-C10	-2.49	119.44	122.92
28	a	410	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
28	d	403	CLA	O2A-CGA-CBA	2.49	119.71	111.91
45	k	101	4RF	O18-C16-C15	2.49	119.71	111.91
28	C	502	CLA	CHA-C4D-ND	2.49	137.70	132.50
28	S	614	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
45	k	101	4RF	O40-C41-C43	2.49	119.71	111.91
28	S	610	CLA	CHA-C4D-ND	2.48	137.70	132.50
46	N	608	CHL	CHB-C4A-NA	2.48	127.95	124.51
28	c	506	CLA	C1-C2-C3	-2.48	121.75	126.04
28	G	612	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
28	b	606	CLA	CHA-C4D-ND	2.48	137.69	132.50
28	b	613	CLA	CHA-C4D-ND	2.48	137.69	132.50
28	S	609	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
28	N	610	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
43	h	101	RRX	C8-C9-C10	-2.48	115.14	118.94
28	C	511	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
30	c	515	BCR	C38-C26-C25	-2.48	121.75	124.53
28	B	607	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
28	B	602	CLA	CHA-C4D-ND	2.48	137.68	132.50
28	C	509	CLA	CHA-C4D-ND	2.48	137.68	132.50
28	b	616	CLA	CHA-C4D-ND	2.48	137.68	132.50
28	G	613	CLA	O2A-CGA-CBA	2.48	119.68	111.91
28	c	503	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
28	Y	612	CLA	CMA-C3A-C4A	2.47	118.42	111.77
32	h	102	LMG	O8-C28-C29	2.47	119.67	111.91
28	C	507	CLA	CMA-C3A-C4A	2.47	118.42	111.77
47	S	621	LUT	C11-C10-C9	-2.47	123.78	127.31
28	Y	612	CLA	CHA-C4D-ND	2.47	137.67	132.50
28	A	407	CLA	CHA-C4D-ND	2.47	137.67	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	606	CLA	CHA-C4D-ND	2.47	137.67	132.50
30	A	411	BCR	C23-C24-C25	-2.47	120.26	127.20
28	C	507	CLA	CMB-C2B-C3B	2.47	129.30	124.68
28	G	602	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
28	b	608	CLA	CHA-C4D-ND	2.47	137.66	132.50
28	c	505	CLA	CHA-C4D-ND	2.47	137.66	132.50
46	G	608	CHL	C4A-NA-C1A	2.47	107.82	106.71
28	b	610	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
47	N	620	LUT	C31-C30-C29	-2.47	123.79	127.31
28	A	405	CLA	CMD-C2D-C3D	-2.47	121.94	127.61
35	B	623	DGD	O1G-C1A-C2A	2.47	119.64	111.91
28	Y	614	CLA	CMA-C3A-C4A	2.46	118.40	111.77
47	G	621	LUT	C38-C25-C24	-2.46	118.28	123.56
30	C	515	BCR	C33-C5-C4	2.46	118.35	113.62
28	b	617	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
28	A	410	CLA	O2A-CGA-CBA	2.46	119.64	111.91
28	c	502	CLA	CHA-C4D-ND	2.46	137.65	132.50
28	C	512	CLA	CHA-C4D-ND	2.46	137.65	132.50
30	a	411	BCR	C36-C18-C17	-2.46	119.48	122.92
28	C	510	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
46	S	606	CHL	CHB-C4A-NA	2.46	127.91	124.51
28	b	612	CLA	O2A-CGA-CBA	2.46	119.63	111.91
28	a	407	CLA	C3D-C2D-C1D	-2.46	102.47	105.83
28	B	616	CLA	CHA-C4D-ND	2.46	137.64	132.50
28	S	613	CLA	CHA-C4D-ND	2.46	137.64	132.50
28	b	602	CLA	CHA-C4D-ND	2.46	137.64	132.50
28	c	501	CLA	CHA-C4D-ND	2.46	137.64	132.50
37	B	625	DGA	OG1-CA1-CA2	2.46	119.62	111.91
28	A	406	CLA	C2D-C1D-ND	2.46	111.92	110.10
47	S	620	LUT	C10-C11-C12	-2.46	115.55	123.22
30	C	517	BCR	C23-C22-C21	2.46	122.71	118.94
28	B	616	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
28	C	507	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
28	S	604	CLA	C2D-C1D-ND	2.45	111.91	110.10
28	B	603	CLA	CHA-C4D-ND	2.45	137.63	132.50
38	Y	624	LHG	O8-C23-C24	2.45	119.61	111.91
28	b	612	CLA	C2C-C1C-NC	2.45	112.27	109.97
28	Y	603	CLA	C1-C2-C3	-2.45	121.80	126.04
28	S	609	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
41	D	405	PL9	C22-C23-C24	-2.45	121.76	127.66
28	G	603	CLA	CHA-C4D-ND	2.45	137.62	132.50
28	Y	614	CLA	O2D-CGD-O1D	-2.45	119.05	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	611	CLA	CHA-C4D-ND	2.45	137.62	132.50
28	Y	612	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
28	a	406	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
30	B	619	BCR	C35-C13-C12	2.45	121.93	118.08
49	N	623	NEX	C38-C25-C26	-2.45	118.16	122.26
28	b	607	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
28	B	612	CLA	CMA-C3A-C4A	2.45	118.35	111.77
28	D	402	CLA	CAC-C3C-C4C	2.45	127.98	124.81
28	C	503	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
28	c	506	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
28	D	403	CLA	C2D-C1D-ND	2.45	111.91	110.10
28	c	509	CLA	CHA-C4D-ND	2.45	137.62	132.50
46	N	606	CHL	C1-C2-C3	-2.45	121.81	126.04
30	C	516	BCR	C31-C1-C6	-2.45	106.33	110.30
28	B	609	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
32	A	413	LMG	O8-C28-C29	2.44	119.58	111.91
28	G	614	CLA	CMD-C2D-C3D	-2.44	121.99	127.61
30	B	619	BCR	C28-C27-C26	-2.44	109.71	114.08
28	B	617	CLA	CMA-C3A-C4A	2.44	118.34	111.77
28	Y	604	CLA	CHA-C4D-ND	2.44	137.61	132.50
28	B	602	CLA	C1-C2-C3	-2.44	121.82	126.04
28	S	604	CLA	CHA-C4D-ND	2.44	137.61	132.50
28	G	603	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
28	b	604	CLA	C1-C2-C3	-2.44	121.82	126.04
46	G	609	CHL	CHD-C4C-C3C	2.44	128.43	124.84
28	B	613	CLA	CHD-C1D-ND	-2.44	122.21	124.45
28	d	403	CLA	CHA-C4D-ND	2.44	137.60	132.50
28	b	611	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
46	Y	601	CHL	C4A-NA-C1A	2.44	107.80	106.71
28	G	613	CLA	CHA-C4D-ND	2.44	137.60	132.50
28	b	607	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
28	b	611	CLA	CHA-C4D-ND	2.44	137.60	132.50
46	N	608	CHL	C4D-CHA-C1A	2.44	124.22	121.25
28	C	503	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
46	G	601	CHL	C1-O2A-CGA	2.44	122.84	116.44
28	B	613	CLA	CMD-C2D-C3D	-2.44	122.01	127.61
28	B	614	CLA	CHA-C4D-ND	2.44	137.59	132.50
28	N	613	CLA	CHA-C4D-ND	2.44	137.59	132.50
28	b	607	CLA	O2A-CGA-CBA	2.44	119.55	111.91
30	d	404	BCR	C36-C18-C17	-2.44	119.51	122.92
28	S	605	CLA	C1-O2A-CGA	2.44	122.83	116.44
28	Y	602	CLA	CHA-C4D-ND	2.44	137.59	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	402	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
28	b	610	CLA	O2A-CGA-CBA	2.43	119.54	111.91
28	Y	612	CLA	C1-C2-C3	-2.43	121.83	126.04
28	c	507	CLA	C2D-C1D-ND	2.43	111.90	110.10
28	c	504	CLA	CHA-C4D-ND	2.43	137.59	132.50
28	B	611	CLA	CHA-C4D-ND	2.43	137.59	132.50
32	C	521	LMG	C8-O7-C10	-2.43	111.80	117.79
28	C	501	CLA	CHA-C4D-ND	2.43	137.59	132.50
28	S	617	CLA	CHA-C4D-ND	2.43	137.59	132.50
28	S	605	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
28	b	617	CLA	CHD-C1D-ND	-2.43	122.22	124.45
29	a	408	PHO	CMC-C2C-C3C	2.43	129.53	124.94
46	N	607	CHL	C1-O2A-CGA	2.43	122.82	116.44
28	c	513	CLA	CHA-C4D-ND	2.43	137.58	132.50
28	B	603	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
28	B	610	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
28	c	510	CLA	CHA-C4D-ND	2.43	137.58	132.50
28	c	511	CLA	CMB-C2B-C3B	2.43	129.22	124.68
28	B	610	CLA	C1-O2A-CGA	2.43	122.82	116.44
30	C	517	BCR	C33-C5-C6	-2.43	121.80	124.53
28	Y	613	CLA	CHA-C4D-ND	2.43	137.58	132.50
30	D	404	BCR	C33-C5-C4	2.43	118.28	113.62
28	S	612	CLA	CHA-C4D-ND	2.43	137.57	132.50
28	Y	614	CLA	CHA-C4D-ND	2.43	137.57	132.50
28	B	617	CLA	CHA-C4D-ND	2.43	137.57	132.50
30	c	515	BCR	C34-C9-C10	-2.43	119.53	122.92
29	A	408	PHO	O2D-CGD-O1D	-2.42	119.10	123.84
28	S	614	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
28	N	602	CLA	C1D-ND-C4D	-2.42	104.61	106.33
28	C	509	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
28	B	612	CLA	O2A-CGA-CBA	2.42	119.51	111.91
46	Y	609	CHL	C1-C2-C3	-2.42	121.85	126.04
28	C	513	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
28	Y	604	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
46	G	607	CHL	C1-C2-C3	-2.42	121.86	126.04
28	a	405	CLA	CHA-C4D-ND	2.42	137.56	132.50
28	D	403	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
29	a	408	PHO	O2D-CGD-O1D	-2.42	119.11	123.84
28	c	511	CLA	CHA-C4D-ND	2.42	137.56	132.50
30	c	514	BCR	C38-C26-C25	-2.42	121.81	124.53
37	b	625	DGA	OG1-CA1-CA2	2.42	119.50	111.91
33	Y	625	SPH	C3-C4-C5	-2.42	119.40	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	511	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
47	Y	621	LUT	C18-C5-C6	-2.42	121.81	124.53
28	b	617	CLA	CHA-C4D-ND	2.41	137.55	132.50
28	b	604	CLA	C2D-C1D-ND	2.41	111.88	110.10
28	S	602	CLA	CHA-C4D-ND	2.41	137.55	132.50
28	Y	611	CLA	CMA-C3A-C4A	2.41	118.26	111.77
30	d	404	BCR	C37-C22-C21	-2.41	119.55	122.92
38	d	408	LHG	O8-C23-C24	2.41	119.47	111.91
46	S	607	CHL	CHB-C4A-NA	2.41	127.84	124.51
28	Y	603	CLA	CHA-C4D-ND	2.41	137.54	132.50
28	A	405	CLA	C2D-C1D-ND	2.41	111.88	110.10
28	B	614	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
28	b	608	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
28	Y	610	CLA	CMA-C3A-C4A	2.41	118.24	111.77
46	G	601	CHL	CHB-C4A-NA	2.40	127.84	124.51
28	c	506	CLA	CHA-C4D-ND	2.40	137.53	132.50
28	N	610	CLA	CMA-C3A-C4A	2.40	118.23	111.77
28	b	612	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
34	B	620	C7Z	C8-C7-C6	-2.40	120.45	127.20
49	S	623	NEX	C1-C2-C3	2.40	119.07	113.64
28	G	602	CLA	CMC-C2C-C1C	2.40	128.70	125.04
28	N	610	CLA	CHA-C4D-ND	2.40	137.53	132.50
46	Y	601	CHL	C1-O2A-CGA	2.40	122.75	116.44
28	N	614	CLA	CHA-C4D-ND	2.40	137.52	132.50
28	c	509	CLA	C2D-C1D-ND	2.40	111.87	110.10
28	C	502	CLA	CMA-C3A-C4A	2.40	118.22	111.77
28	b	606	CLA	O2A-CGA-CBA	2.40	119.44	111.91
28	d	402	CLA	CHA-C4D-ND	2.40	137.52	132.50
46	N	609	CHL	C2C-C3C-C4C	2.40	108.20	106.49
28	b	607	CLA	CAA-C2A-C3A	-2.40	106.22	112.78
28	b	603	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
28	S	609	CLA	CHA-C4D-ND	2.40	137.51	132.50
28	G	614	CLA	CHA-C4D-ND	2.39	137.51	132.50
28	C	503	CLA	O2A-CGA-CBA	2.39	119.42	111.91
28	c	511	CLA	O2A-CGA-CBA	2.39	119.42	111.91
30	B	619	BCR	C4-C5-C6	-2.39	119.26	122.73
28	N	614	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
28	B	606	CLA	C1D-ND-C4D	-2.39	104.64	106.33
28	c	509	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
28	Y	610	CLA	CHA-C4D-ND	2.39	137.50	132.50
28	a	406	CLA	CHA-C1A-NA	-2.39	120.93	126.40
28	c	511	CLA	CHA-C1A-NA	-2.39	120.93	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	615	CLA	CMB-C2B-C1B	-2.39	124.80	128.46
46	G	607	CHL	C4D-CHA-C1A	2.39	124.15	121.25
28	c	509	CLA	CMB-C2B-C3B	2.39	129.14	124.68
28	c	505	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
28	Y	603	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
47	G	621	LUT	C10-C11-C12	-2.38	115.78	123.22
28	b	608	CLA	CMB-C2B-C3B	2.38	129.14	124.68
28	c	513	CLA	CHA-C1A-NA	-2.38	120.94	126.40
28	c	509	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
28	B	604	CLA	CMD-C2D-C3D	-2.38	122.13	127.61
28	A	410	CLA	CHA-C4D-ND	2.38	137.48	132.50
28	C	505	CLA	CHD-C1D-ND	-2.38	122.27	124.45
28	B	617	CLA	C1-O2A-CGA	2.38	122.69	116.44
28	c	503	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
28	A	406	CLA	CHA-C4D-ND	2.38	137.47	132.50
28	D	403	CLA	CHA-C4D-ND	2.38	137.47	132.50
28	b	603	CLA	CHA-C4D-ND	2.38	137.47	132.50
28	C	507	CLA	CHA-C1A-NA	-2.38	120.95	126.40
28	S	613	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
28	N	604	CLA	CMA-C3A-C4A	2.38	118.16	111.77
30	C	517	BCR	C38-C26-C25	-2.38	121.86	124.53
28	D	402	CLA	CAA-CBA-CGA	-2.38	106.31	113.25
28	C	508	CLA	CHA-C4D-ND	2.37	137.47	132.50
42	F	101	HEM	C1B-NB-C4B	2.37	107.53	105.07
30	b	618	BCR	C30-C25-C26	-2.37	119.27	122.61
28	Y	613	CLA	C1-C2-C3	-2.37	121.94	126.04
28	B	605	CLA	CMD-C2D-C3D	-2.37	122.15	127.61
46	N	606	CHL	C1-O2A-CGA	2.37	122.67	116.44
46	G	601	CHL	C1-C2-C3	-2.37	121.94	126.04
28	C	504	CLA	CHA-C4D-ND	2.37	137.46	132.50
28	G	610	CLA	CHA-C4D-ND	2.37	137.46	132.50
34	b	620	C7Z	C22-C23-C24	2.37	113.55	110.30
28	Y	604	CLA	CMA-C3A-C4A	2.37	118.15	111.77
30	c	516	BCR	C37-C22-C21	-2.37	119.60	122.92
28	B	610	CLA	CHA-C4D-ND	2.37	137.46	132.50
28	d	402	CLA	C1D-ND-C4D	-2.37	104.65	106.33
34	b	620	C7Z	C31-C32-C33	-2.37	119.76	126.42
28	B	612	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
46	N	605	CHL	C1-O2A-CGA	2.37	122.66	116.44
28	A	405	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
28	C	509	CLA	CMA-C3A-C4A	2.37	118.14	111.77
28	G	614	CLA	O2A-CGA-CBA	2.37	119.33	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	G	607	CHL	C1B-CHB-C4A	-2.36	125.44	130.12
28	Y	613	CLA	C1-O2A-CGA	2.36	122.64	116.44
28	G	602	CLA	CHA-C4D-ND	2.36	137.44	132.50
47	G	621	LUT	C31-C30-C29	-2.36	123.94	127.31
28	C	509	CLA	C2D-C1D-ND	2.36	111.84	110.10
31	B	626	SQD	O3-C3-C2	-2.36	104.89	110.35
28	N	602	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
28	c	503	CLA	CHA-C1A-NA	-2.36	120.99	126.40
28	b	605	CLA	C1-C2-C3	-2.36	121.96	126.04
28	A	407	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
28	c	505	CLA	CMB-C2B-C3B	2.36	129.09	124.68
47	G	620	LUT	C10-C11-C12	-2.36	115.85	123.22
28	C	512	CLA	CHD-C1D-ND	-2.36	122.29	124.45
28	B	606	CLA	O2A-CGA-CBA	2.36	119.30	111.91
48	Y	622	XAT	C6-C7-C8	-2.36	121.01	125.99
28	C	507	CLA	OBD-CAD-C3D	-2.35	122.85	128.52
28	a	407	CLA	C1C-C2C-C3C	-2.35	104.48	106.96
46	G	609	CHL	C3C-C4C-NC	-2.35	107.93	110.57
28	B	607	CLA	C2D-C1D-ND	2.35	111.84	110.10
28	b	605	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
28	a	407	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
28	S	614	CLA	C2D-C1D-ND	2.35	111.84	110.10
28	c	503	CLA	CHA-C4D-ND	2.35	137.42	132.50
28	b	614	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
28	Y	602	CLA	CMB-C2B-C3B	2.35	129.08	124.68
30	C	514	BCR	C36-C18-C17	-2.35	119.63	122.92
28	S	610	CLA	O2A-CGA-CBA	2.35	119.28	111.91
46	N	609	CHL	CHB-C4A-NA	2.35	127.76	124.51
30	C	514	BCR	C34-C9-C10	-2.35	119.63	122.92
28	S	617	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
28	c	506	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
28	N	602	CLA	CHA-C4D-ND	2.35	137.41	132.50
28	B	612	CLA	CHA-C4D-ND	2.35	137.41	132.50
28	C	506	CLA	O2A-CGA-CBA	2.35	119.27	111.91
30	B	618	BCR	C36-C18-C17	-2.35	119.64	122.92
48	Y	622	XAT	C19-C9-C10	-2.35	119.64	122.92
28	b	611	CLA	C3D-C2D-C1D	-2.34	102.63	105.83
28	G	603	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
28	B	610	CLA	C1C-C2C-C3C	-2.34	104.49	106.96
46	S	601	CHL	C4A-NA-C1A	2.34	107.76	106.71
46	S	606	CHL	C1B-CHB-C4A	-2.34	125.48	130.12
28	B	607	CLA	CMD-C2D-C3D	-2.34	122.23	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	613	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
46	G	608	CHL	CHB-C4A-NA	2.34	127.75	124.51
49	S	623	NEX	C26-C27-C28	-2.34	121.05	125.99
28	c	507	CLA	CHA-C1A-NA	-2.34	121.04	126.40
30	A	411	BCR	C19-C18-C17	2.34	122.53	118.94
28	B	614	CLA	O2A-CGA-CBA	2.34	119.25	111.91
28	b	614	CLA	CMB-C2B-C1B	-2.34	124.87	128.46
28	B	605	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
28	a	405	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
32	h	102	LMG	O1-C1-C2	2.34	111.95	108.30
28	b	615	CLA	CMB-C2B-C1B	-2.34	124.87	128.46
28	c	510	CLA	O2A-CGA-CBA	2.34	119.24	111.91
28	b	604	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
28	b	610	CLA	CMB-C2B-C1B	-2.34	124.88	128.46
28	S	613	CLA	CMD-C2D-C3D	-2.33	122.24	127.61
30	c	515	BCR	C1-C6-C7	2.33	122.38	115.78
30	C	515	BCR	C15-C14-C13	-2.33	123.98	127.31
28	b	609	CLA	CMA-C3A-C4A	2.33	118.04	111.77
46	N	607	CHL	C1-C2-C3	-2.33	122.01	126.04
28	A	407	CLA	O2A-CGA-CBA	2.33	119.22	111.91
43	h	101	RRX	C36-C18-C19	2.33	121.75	118.08
28	C	501	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
46	Y	609	CHL	CHB-C4A-NA	2.33	127.73	124.51
28	Y	610	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
47	S	620	LUT	C39-C29-C28	2.33	121.74	118.08
30	b	618	BCR	C4-C5-C6	-2.33	119.36	122.73
28	a	405	CLA	CMB-C2B-C1B	-2.32	124.89	128.46
49	S	623	NEX	C4-C3-C2	2.32	115.26	110.77
46	N	607	CHL	CMB-C2B-C1B	-2.32	124.90	128.46
28	b	617	CLA	CMB-C2B-C3B	2.32	129.02	124.68
47	G	621	LUT	C18-C5-C6	-2.32	121.92	124.53
47	S	620	LUT	C30-C31-C32	-2.32	115.98	123.22
34	b	620	C7Z	C2-C3-C4	2.32	113.48	110.30
31	c	526	SQD	O3-C3-C2	-2.32	104.99	110.35
28	S	602	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
46	S	608	CHL	C4A-NA-C1A	2.32	107.75	106.71
28	C	501	CLA	C1D-ND-C4D	-2.32	104.69	106.33
47	S	621	LUT	C39-C29-C28	2.32	121.73	118.08
42	F	101	HEM	CAD-CBD-CGD	-2.32	108.62	113.60
46	N	606	CHL	C4A-NA-C1A	2.32	107.75	106.71
48	Y	622	XAT	O24-C25-C38	-2.32	112.28	115.06
28	c	513	CLA	O2D-CGD-O1D	-2.31	119.31	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	403	CLA	CHA-C1A-NA	-2.31	121.10	126.40
32	H	102	LMG	O8-C28-C29	2.31	119.17	111.91
28	Y	614	CLA	C1-C2-C3	-2.31	122.04	126.04
28	C	509	CLA	CMB-C2B-C3B	2.31	129.00	124.68
28	B	614	CLA	CMB-C2B-C3B	2.31	129.00	124.68
28	G	610	CLA	CMA-C3A-C4A	2.31	117.98	111.77
28	B	606	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
28	Y	614	CLA	O2A-CGA-CBA	2.31	119.16	111.91
28	S	612	CLA	C1D-ND-C4D	-2.31	104.69	106.33
31	b	626	SQD	O3-C3-C2	-2.31	105.01	110.35
30	c	516	BCR	C35-C13-C14	-2.31	119.69	122.92
28	S	614	CLA	CMB-C2B-C3B	2.31	128.99	124.68
28	C	502	CLA	C1C-C2C-C3C	-2.30	104.53	106.96
28	c	507	CLA	OBD-CAD-C3D	-2.30	122.97	128.52
28	C	505	CLA	CMB-C2B-C1B	-2.30	124.92	128.46
28	S	614	CLA	O2A-CGA-CBA	2.30	119.14	111.91
28	Y	613	CLA	CMD-C2D-C3D	-2.30	122.31	127.61
28	C	504	CLA	C1D-ND-C4D	-2.30	104.70	106.33
28	a	407	CLA	C1D-ND-C4D	-2.30	104.70	106.33
28	S	612	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
28	S	602	CLA	C1D-ND-C4D	-2.30	104.70	106.33
28	N	610	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
49	Y	623	NEX	C19-C9-C10	-2.30	119.70	122.92
46	G	607	CHL	C3C-C4C-NC	-2.30	107.99	110.57
28	c	501	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
28	B	611	CLA	CHA-C1A-NA	-2.30	121.13	126.40
28	G	614	CLA	CMB-C2B-C3B	2.30	128.98	124.68
28	B	615	CLA	CMA-C3A-C4A	2.30	117.95	111.77
30	B	619	BCR	C36-C18-C17	-2.30	119.70	122.92
49	G	623	NEX	C4-C3-C2	2.30	115.21	110.77
35	b	623	DGD	O6D-C5D-C6D	2.30	111.30	106.67
49	S	623	NEX	C20-C13-C14	-2.30	119.71	122.92
41	d	405	PL9	C32-C33-C34	-2.29	122.14	127.66
30	c	517	BCR	C19-C18-C17	2.29	122.46	118.94
31	M	101	SQD	O3-C3-C2	-2.29	105.05	110.35
31	C	526	SQD	O3-C3-C2	-2.29	105.05	110.35
46	N	608	CHL	CMB-C2B-C1B	-2.29	124.94	128.46
28	C	504	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
28	B	616	CLA	CHA-C1A-NA	-2.29	121.15	126.40
28	b	607	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
28	Y	603	CLA	C1D-ND-C4D	-2.29	104.71	106.33
28	Y	608	CLA	O2D-CGD-O1D	-2.29	119.36	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Y	602	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
31	m	101	SQD	O3-C3-C2	-2.29	105.06	110.35
28	b	612	CLA	CHA-C4D-ND	2.29	137.29	132.50
31	b	621	SQD	O3-C3-C2	-2.29	105.06	110.35
28	C	513	CLA	CHA-C4D-ND	2.29	137.28	132.50
28	a	406	CLA	C2A-C1A-CHA	2.29	127.86	123.86
28	b	616	CLA	C1-O2A-CGA	2.29	122.44	116.44
28	a	405	CLA	C2C-C1C-NC	2.29	112.11	109.97
31	a	412	SQD	O3-C3-C2	-2.28	105.07	110.35
46	N	609	CHL	CMB-C2B-C1B	-2.28	124.95	128.46
46	G	607	CHL	CMB-C2B-C1B	-2.28	124.96	128.46
28	b	603	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
28	Y	610	CLA	C1D-ND-C4D	-2.28	104.71	106.33
28	Y	608	CLA	CHA-C1A-NA	-2.28	121.17	126.40
48	N	622	XAT	C18-C5-C6	-2.28	118.44	122.26
28	N	614	CLA	CHA-C1A-NA	-2.28	121.17	126.40
28	D	403	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
28	S	614	CLA	CHA-C1A-NA	-2.28	121.18	126.40
28	C	503	CLA	CMB-C2B-C3B	2.28	128.94	124.68
28	A	406	CLA	O2A-CGA-CBA	2.28	119.06	111.91
28	N	612	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
28	b	602	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
28	c	503	CLA	C1D-ND-C4D	-2.28	104.72	106.33
43	h	101	RRX	C20-C21-C22	2.27	130.56	127.31
46	Y	606	CHL	C4D-CHA-C1A	2.27	124.02	121.25
47	Y	621	LUT	C10-C11-C12	-2.27	116.12	123.22
49	Y	623	NEX	C26-C27-C28	-2.27	121.19	125.99
41	D	405	PL9	C20-C19-C21	2.27	119.09	115.27
28	c	502	CLA	CMB-C2B-C1B	-2.27	124.97	128.46
28	B	609	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
28	C	504	CLA	C1-O2A-CGA	2.27	122.40	116.44
28	S	604	CLA	C1-C2-C3	-2.27	122.11	126.04
48	G	622	XAT	O4-C5-C18	-2.27	112.33	115.06
28	C	511	CLA	CHA-C1A-NA	-2.27	121.20	126.40
30	c	514	BCR	C34-C9-C10	-2.27	119.74	122.92
43	H	101	RRX	C35-C13-C14	-2.27	119.74	122.92
28	N	604	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
28	Y	613	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
28	N	612	CLA	CHA-C1A-NA	-2.27	121.20	126.40
28	c	506	CLA	O2A-CGA-CBA	2.27	119.03	111.91
28	b	603	CLA	O2A-CGA-CBA	2.27	119.03	111.91
28	G	612	CLA	CMA-C3A-C4A	2.27	117.87	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	611	CLA	O2A-CGA-CBA	2.27	119.02	111.91
46	Y	601	CHL	CMB-C2B-C1B	-2.27	124.98	128.46
46	N	601	CHL	C1-O2A-CGA	2.27	122.39	116.44
28	N	610	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
38	c	525	LHG	C5-O7-C7	-2.26	112.22	117.79
28	G	614	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
30	B	619	BCR	C34-C9-C10	-2.26	119.75	122.92
28	b	604	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
46	G	607	CHL	CHC-C1C-NC	2.26	127.64	124.20
28	G	610	CLA	C1D-ND-C4D	-2.26	104.73	106.33
30	D	404	BCR	C37-C22-C21	-2.26	119.75	122.92
28	B	608	CLA	O2A-CGA-CBA	2.26	119.00	111.91
28	b	605	CLA	C2D-C1D-ND	2.26	111.77	110.10
28	a	406	CLA	O2A-CGA-CBA	2.26	119.00	111.91
30	b	618	BCR	C23-C24-C25	-2.26	120.86	127.20
46	Y	607	CHL	CMB-C2B-C1B	-2.26	124.99	128.46
28	b	617	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
32	c	523	LMG	C8-O7-C10	-2.26	112.23	117.79
28	S	604	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
28	Y	612	CLA	CHA-C1A-NA	-2.26	121.23	126.40
28	C	501	CLA	O2A-CGA-CBA	2.26	118.99	111.91
31	B	621	SQD	O3-C3-C2	-2.26	105.13	110.35
28	b	606	CLA	CMA-C3A-C4A	2.26	117.84	111.77
30	B	618	BCR	C8-C7-C6	-2.26	120.87	127.20
28	b	611	CLA	CHA-C1A-NA	-2.26	121.23	126.40
31	A	412	SQD	O3-C3-C2	-2.26	105.13	110.35
28	Y	604	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
49	S	623	NEX	C17-C1-C6	-2.25	108.45	110.47
28	a	406	CLA	C2D-C1D-ND	2.25	111.76	110.10
28	G	613	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
28	c	513	CLA	C1D-ND-C4D	-2.25	104.73	106.33
28	C	503	CLA	CHA-C1A-NA	-2.25	121.24	126.40
28	B	604	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
28	B	617	CLA	CHD-C1D-ND	-2.25	122.39	124.45
30	C	514	BCR	C33-C5-C4	2.25	117.94	113.62
28	c	504	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
41	D	405	PL9	C27-C28-C29	-2.25	122.24	127.66
42	f	101	HEM	C1B-NB-C4B	2.25	107.40	105.07
28	b	608	CLA	O2A-CGA-CBA	2.25	118.97	111.91
28	c	504	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
46	S	601	CHL	C1B-CHB-C4A	-2.25	125.66	130.12
28	C	511	CLA	CAA-CBA-CGA	-2.25	106.68	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	604	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
28	d	403	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
28	Y	610	CLA	CMB-C2B-C3B	2.25	128.88	124.68
28	G	611	CLA	C2D-C1D-ND	2.25	111.76	110.10
28	G	614	CLA	C1D-ND-C4D	-2.25	104.74	106.33
43	H	101	RRX	C2-C1-C6	2.24	113.94	110.48
28	N	613	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
46	Y	609	CHL	C4D-CHA-C1A	2.24	123.98	121.25
28	d	403	CLA	CMA-C3A-C2A	2.24	122.87	113.83
28	S	602	CLA	CMB-C2B-C3B	2.24	128.87	124.68
28	c	508	CLA	CAC-C3C-C4C	2.24	127.72	124.81
47	S	621	LUT	C31-C32-C33	-2.24	120.13	126.42
48	Y	622	XAT	C40-C33-C34	-2.24	119.79	122.92
43	h	101	RRX	C19-C18-C17	-2.24	115.51	118.94
28	B	614	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
28	N	614	CLA	C1D-ND-C4D	-2.24	104.75	106.33
28	b	603	CLA	C1D-ND-C4D	-2.23	104.75	106.33
28	c	513	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
28	B	605	CLA	C2D-C1D-ND	2.23	111.75	110.10
28	b	616	CLA	CHA-C1A-NA	-2.23	121.28	126.40
28	c	505	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
28	b	602	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
28	c	502	CLA	CHA-C1A-NA	-2.23	121.29	126.40
28	C	503	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
28	B	611	CLA	O2A-CGA-CBA	2.23	118.90	111.91
28	b	616	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
28	C	513	CLA	CHA-C1A-NA	-2.23	121.30	126.40
28	c	503	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
28	c	511	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
28	D	402	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
30	c	514	BCR	C37-C22-C21	-2.23	119.81	122.92
28	b	616	CLA	CMA-C3A-C4A	2.23	117.75	111.77
28	a	410	CLA	CHA-C1A-NA	-2.23	121.30	126.40
47	N	620	LUT	C10-C11-C12	-2.23	116.27	123.22
28	C	509	CLA	C1-C2-C3	-2.22	122.19	126.04
30	b	619	BCR	C34-C9-C10	-2.22	119.81	122.92
28	N	604	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
28	C	506	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
28	b	602	CLA	CHA-C1A-NA	-2.22	121.31	126.40
28	c	513	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
28	G	612	CLA	CHA-C1A-NA	-2.22	121.31	126.40
28	b	614	CLA	CHA-C1A-NA	-2.22	121.31	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	605	CLA	CHA-C1A-NA	-2.22	121.31	126.40
28	b	607	CLA	CMB-C2B-C3B	2.22	128.83	124.68
28	B	604	CLA	C2D-C1D-ND	2.22	111.74	110.10
46	N	607	CHL	C4A-NA-C1A	2.22	107.70	106.71
41	D	405	PL9	C40-C39-C41	2.22	119.00	115.27
28	c	508	CLA	CHA-C4D-ND	2.22	137.14	132.50
30	A	411	BCR	C34-C9-C10	-2.22	119.81	122.92
28	c	501	CLA	O2A-CGA-CBA	2.22	118.86	111.91
28	B	607	CLA	CMB-C2B-C1B	-2.22	125.06	128.46
28	B	605	CLA	CHA-C1A-NA	-2.22	121.32	126.40
28	B	610	CLA	CHA-C1A-NA	-2.22	121.32	126.40
28	N	603	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
28	N	610	CLA	C1D-ND-C4D	-2.21	104.76	106.33
28	B	602	CLA	O2A-CGA-CBA	2.21	118.86	111.91
28	c	510	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
28	S	603	CLA	CHA-C1A-NA	-2.21	121.33	126.40
28	G	603	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
28	B	615	CLA	C2D-C1D-ND	2.21	111.73	110.10
28	c	501	CLA	C1D-ND-C4D	-2.21	104.76	106.33
28	C	510	CLA	O2A-CGA-CBA	2.21	118.85	111.91
28	a	407	CLA	CHA-C1A-NA	-2.21	121.34	126.40
28	D	402	CLA	CHD-C1D-ND	-2.21	122.42	124.45
28	b	611	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
28	c	511	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
28	S	611	CLA	CHA-C1A-NA	-2.21	121.34	126.40
28	Y	604	CLA	O2A-CGA-CBA	2.21	118.83	111.91
41	d	405	PL9	C26-C24-C23	-2.21	116.65	121.12
46	G	609	CHL	CHB-C4A-NA	2.20	127.56	124.51
35	B	623	DGD	O2G-C1B-O1B	-2.20	118.38	123.70
28	G	612	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
28	B	617	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
34	b	620	C7Z	C20-C13-C14	-2.20	119.84	122.92
28	c	502	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
30	c	516	BCR	C38-C26-C25	-2.20	122.06	124.53
28	G	611	CLA	O2A-CGA-CBA	2.20	118.80	111.91
28	Y	602	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
28	b	613	CLA	CHA-C1A-NA	-2.20	121.37	126.40
28	A	405	CLA	CHA-C1A-NA	-2.20	121.37	126.40
28	b	608	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
28	G	603	CLA	C1D-ND-C4D	-2.19	104.78	106.33
28	B	608	CLA	C2D-C1D-ND	2.19	111.72	110.10
28	N	602	CLA	CMD-C2D-C3D	-2.19	122.57	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	Y	627	PTY	C6-O7-C8	-2.19	113.81	117.90
28	C	507	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
28	C	512	CLA	C1-O2A-CGA	2.19	122.19	116.44
28	G	611	CLA	CHA-C1A-NA	-2.19	121.38	126.40
28	G	604	CLA	OBD-CAD-C3D	-2.19	123.25	128.52
28	b	605	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
28	Y	603	CLA	O2A-CGA-CBA	2.19	118.78	111.91
28	B	614	CLA	C1D-ND-C4D	-2.19	104.78	106.33
28	b	606	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
47	S	621	LUT	C10-C11-C12	-2.19	116.39	123.22
28	D	402	CLA	CMC-C2C-C1C	2.19	128.37	125.04
30	C	516	BCR	C8-C9-C10	2.19	122.30	118.94
46	G	601	CHL	C4D-CHA-C1A	2.19	123.91	121.25
28	N	611	CLA	CHA-C1A-NA	-2.19	121.39	126.40
49	N	623	NEX	C31-C30-C29	2.19	130.43	127.31
40	D	401	BCT	O3-C-O1	-2.18	113.88	119.55
46	G	601	CHL	C1B-CHB-C4A	-2.18	125.79	130.12
28	A	406	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
28	Y	608	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
49	N	623	NEX	C20-C13-C14	-2.18	119.86	122.92
46	Y	609	CHL	CHD-C4C-C3C	2.18	128.05	124.84
28	b	610	CLA	C1D-ND-C4D	-2.18	104.78	106.33
30	c	514	BCR	C33-C5-C4	2.18	117.81	113.62
28	b	617	CLA	C1-O2A-CGA	2.18	122.17	116.44
30	D	404	BCR	C33-C5-C6	-2.18	122.08	124.53
28	S	613	CLA	C1D-ND-C4D	-2.18	104.79	106.33
46	Y	606	CHL	C1B-CHB-C4A	-2.18	125.80	130.12
28	N	611	CLA	O2A-CGA-CBA	2.18	118.74	111.91
28	B	607	CLA	CMA-C3A-C4A	2.18	117.63	111.77
28	Y	611	CLA	CMB-C2B-C3B	2.18	128.75	124.68
28	N	611	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
28	B	614	CLA	CHA-C1A-NA	-2.18	121.42	126.40
28	d	403	CLA	CMB-C2B-C3B	2.18	128.75	124.68
28	G	611	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
28	G	602	CLA	O2A-CGA-CBA	2.17	118.72	111.91
28	N	613	CLA	C1D-ND-C4D	-2.17	104.79	106.33
28	S	613	CLA	C1-O2A-CGA	2.17	122.14	116.44
34	b	620	C7Z	C1-C6-C7	2.17	121.92	115.78
30	C	515	BCR	C38-C26-C25	-2.17	122.09	124.53
30	d	404	BCR	C30-C25-C24	2.17	121.92	115.78
28	B	609	CLA	C1D-ND-C4D	-2.17	104.79	106.33
28	B	603	CLA	CMD-C2D-C3D	-2.17	122.62	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	607	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
46	Y	606	CHL	CHB-C4A-NA	2.17	127.51	124.51
28	S	617	CLA	CHA-C1A-NA	-2.17	121.43	126.40
28	B	612	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
28	B	602	CLA	CHA-C1A-NA	-2.17	121.44	126.40
28	b	603	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
28	S	604	CLA	CMA-C3A-C4A	2.17	117.59	111.77
28	C	502	CLA	CHA-C1A-NA	-2.17	121.44	126.40
28	c	504	CLA	CHA-C1A-NA	-2.17	121.44	126.40
28	C	505	CLA	C1-O2A-CGA	2.17	122.12	116.44
30	d	404	BCR	C34-C9-C10	-2.17	119.89	122.92
28	G	604	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
28	C	506	CLA	C2D-C1D-ND	2.16	111.70	110.10
28	b	609	CLA	CHA-C1A-NA	-2.16	121.44	126.40
28	Y	614	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
28	S	612	CLA	CHA-C1A-NA	-2.16	121.44	126.40
34	B	620	C7Z	C4-C5-C6	-2.16	116.03	120.85
30	C	517	BCR	C31-C1-C6	-2.16	106.79	110.30
28	S	610	CLA	CHA-C1A-NA	-2.16	121.44	126.40
28	a	405	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
28	B	617	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
28	c	502	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
28	Y	613	CLA	C1D-ND-C4D	-2.16	104.80	106.33
46	N	606	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
28	c	503	CLA	O2A-CGA-CBA	2.16	118.69	111.91
30	c	517	BCR	C38-C26-C27	2.16	117.77	113.62
28	c	510	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
48	N	622	XAT	C39-C29-C30	-2.16	119.90	122.92
43	H	101	RRX	C19-C18-C17	-2.16	115.63	118.94
28	A	407	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
46	G	608	CHL	CMB-C2B-C1B	-2.16	125.15	128.46
35	b	623	DGD	C4D-C3D-C2D	2.16	114.59	110.82
28	C	501	CLA	CHA-C1A-NA	-2.16	121.45	126.40
28	b	607	CLA	CHA-C1A-NA	-2.16	121.45	126.40
41	D	405	PL9	O1-C4-C3	-2.16	118.34	120.72
38	d	410	LHG	C5-O7-C7	-2.16	112.48	117.79
28	b	614	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
28	S	610	CLA	C1D-ND-C4D	-2.16	104.80	106.33
28	B	603	CLA	CHA-C1A-NA	-2.16	121.46	126.40
28	c	513	CLA	C2A-C1A-CHA	2.16	127.63	123.86
48	Y	622	XAT	C26-C27-C28	-2.16	121.44	125.99
28	B	602	CLA	C1D-ND-C4D	-2.16	104.80	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	N	603	CLA	CHA-C1A-NA	-2.15	121.46	126.40
28	c	509	CLA	CHA-C1A-NA	-2.15	121.46	126.40
28	C	506	CLA	CHA-C1A-NA	-2.15	121.47	126.40
28	N	604	CLA	CHA-C1A-NA	-2.15	121.47	126.40
46	N	601	CHL	C1B-CHB-C4A	-2.15	125.85	130.12
38	S	624	LHG	C5-O7-C7	-2.15	112.49	117.79
41	D	405	PL9	C31-C32-C33	-2.15	104.81	111.88
34	b	620	C7Z	C8-C7-C6	-2.15	121.16	127.20
28	b	616	CLA	C1D-ND-C4D	-2.15	104.81	106.33
28	c	506	CLA	CHA-C1A-NA	-2.15	121.47	126.40
28	c	512	CLA	CHA-C1A-NA	-2.15	121.47	126.40
49	N	623	NEX	C40-C33-C34	-2.15	119.91	122.92
48	G	622	XAT	C19-C9-C10	-2.15	119.91	122.92
28	S	610	CLA	C1C-C2C-C3C	-2.15	104.69	106.96
28	S	610	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
28	C	508	CLA	CAC-C3C-C4C	2.15	127.60	124.81
28	N	611	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
28	b	617	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
28	c	505	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
28	B	614	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
28	c	508	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
28	Y	603	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
38	N	624	LHG	C5-O7-C7	-2.15	112.51	117.79
28	S	609	CLA	C1D-ND-C4D	-2.15	104.81	106.33
46	G	605	CHL	CMB-C2B-C1B	-2.15	125.17	128.46
28	d	402	CLA	CMA-C3A-C4A	2.14	117.54	111.77
28	B	602	CLA	CMD-C2D-C3D	-2.14	122.68	127.61
28	Y	611	CLA	CHA-C1A-NA	-2.14	121.49	126.40
46	S	607	CHL	C4D-CHA-C1A	2.14	123.86	121.25
30	c	514	BCR	C23-C24-C25	-2.14	121.18	127.20
28	Y	603	CLA	CHA-C1A-NA	-2.14	121.49	126.40
28	G	614	CLA	CHA-C1A-NA	-2.14	121.49	126.40
28	c	510	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
28	a	405	CLA	CMC-C2C-C1C	2.14	128.30	125.04
46	G	605	CHL	C1-O2A-CGA	2.14	122.95	116.73
28	c	501	CLA	CHA-C1A-NA	-2.14	121.50	126.40
28	B	604	CLA	CHA-C1A-NA	-2.14	121.50	126.40
46	N	608	CHL	C4A-NA-C1A	2.14	107.67	106.71
30	B	619	BCR	C27-C26-C25	-2.14	119.63	122.73
28	b	610	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
48	Y	622	XAT	O4-C5-C4	-2.14	111.78	113.38
28	Y	610	CLA	CMD-C2D-C3D	-2.14	122.70	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	612	CLA	CAA-C2A-C3A	-2.14	106.93	112.78
41	d	405	PL9	C36-C34-C33	-2.13	116.80	121.12
38	L	101	LHG	C5-O7-C7	-2.13	112.54	117.79
28	B	617	CLA	CHA-C1A-NA	-2.13	121.51	126.40
28	b	615	CLA	CMA-C3A-C4A	2.13	117.51	111.77
28	C	512	CLA	CHA-C1A-NA	-2.13	121.51	126.40
28	Y	608	CLA	O2A-CGA-CBA	2.13	118.60	111.91
46	N	609	CHL	C1-C2-C3	-2.13	122.36	126.04
28	b	604	CLA	CHA-C1A-NA	-2.13	121.52	126.40
46	G	609	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
28	S	604	CLA	CHA-C1A-NA	-2.13	121.52	126.40
28	C	506	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
28	Y	614	CLA	C1D-ND-C4D	-2.13	104.82	106.33
28	S	609	CLA	CHA-C1A-NA	-2.13	121.52	126.40
46	Y	606	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
28	N	614	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
28	A	405	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
28	C	508	CLA	O2A-CGA-CBA	2.13	118.59	111.91
30	D	404	BCR	C4-C5-C6	-2.13	119.64	122.73
28	C	512	CLA	C1-C2-C3	-2.13	122.36	126.04
28	N	612	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
46	N	601	CHL	C4D-CHA-C1A	2.13	123.84	121.25
28	b	606	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
28	C	513	CLA	C1D-ND-C4D	-2.13	104.82	106.33
28	c	509	CLA	O2A-CGA-CBA	2.13	118.59	111.91
28	G	613	CLA	CHA-C1A-NA	-2.13	121.53	126.40
28	Y	611	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
28	G	603	CLA	O2A-CGA-CBA	2.13	118.58	111.91
46	S	601	CHL	C4D-CHA-C1A	2.13	123.84	121.25
33	A	414	SPH	C3-C4-C5	-2.13	120.05	124.79
28	S	609	CLA	C1-C2-C3	-2.13	122.37	126.04
46	G	606	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
28	B	603	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
28	B	617	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
29	A	408	PHO	C1-C2-C3	-2.12	122.37	126.04
28	B	603	CLA	C1D-ND-C4D	-2.12	104.83	106.33
28	Y	604	CLA	C1D-ND-C4D	-2.12	104.83	106.33
28	c	511	CLA	C1D-ND-C4D	-2.12	104.83	106.33
34	b	620	C7Z	C38-C25-C24	2.12	118.28	114.36
34	b	620	C7Z	C11-C12-C13	-2.12	120.46	126.42
28	b	614	CLA	CMA-C3A-C4A	2.12	117.47	111.77
28	N	613	CLA	CMD-C2D-C3D	-2.12	122.73	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	507	CLA	C1-C2-C3	-2.12	122.38	126.04
48	Y	622	XAT	O4-C5-C18	-2.12	112.52	115.06
28	S	610	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
28	N	612	CLA	CMA-C3A-C4A	2.12	117.47	111.77
28	c	512	CLA	C1-O2A-CGA	2.12	122.01	116.44
28	a	405	CLA	C1C-C2C-C3C	-2.12	104.73	106.96
41	D	405	PL9	O2-C1-C6	2.12	124.26	120.59
28	Y	603	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
28	b	614	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
41	d	405	PL9	O2-C1-C6	2.12	124.26	120.59
46	G	608	CHL	C1B-CHB-C4A	-2.12	125.92	130.12
46	S	606	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
28	A	405	CLA	CAC-C3C-C4C	2.12	127.56	124.81
28	S	602	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
28	C	508	CLA	CHA-C1A-NA	-2.12	121.55	126.40
28	C	505	CLA	CMD-C2D-C3D	-2.12	122.75	127.61
46	N	601	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
46	G	601	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
28	c	512	CLA	C2A-C1A-CHA	2.12	127.56	123.86
28	Y	602	CLA	C1D-ND-C4D	-2.12	104.83	106.33
28	b	614	CLA	O2A-CGA-CBA	2.12	118.55	111.91
30	b	618	BCR	C29-C28-C27	2.11	116.10	111.38
28	N	610	CLA	CHA-C1A-NA	-2.11	121.56	126.40
28	G	610	CLA	C6-C5-C3	-2.11	107.92	113.45
28	N	604	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
46	G	601	CHL	CHD-C4C-C3C	2.11	127.94	124.84
46	Y	609	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
28	C	504	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
28	G	603	CLA	CHA-C1A-NA	-2.11	121.57	126.40
28	G	610	CLA	CMB-C2B-C3B	2.11	128.62	124.68
28	B	612	CLA	C1D-ND-C4D	-2.11	104.84	106.33
28	Y	614	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
43	h	101	RRX	C16-C15-C14	-2.11	119.16	123.47
46	S	601	CHL	CMB-C2B-C1B	-2.11	125.23	128.46
28	G	610	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
28	c	509	CLA	CMB-C2B-C1B	-2.11	125.23	128.46
46	S	607	CHL	CMB-C2B-C1B	-2.11	125.23	128.46
46	S	608	CHL	CMB-C2B-C1B	-2.11	125.23	128.46
46	G	608	CHL	C4D-CHA-C1A	2.11	123.81	121.25
28	S	602	CLA	CHA-C1A-NA	-2.11	121.58	126.40
28	D	402	CLA	CHA-C1A-NA	-2.10	121.58	126.40
28	B	615	CLA	CHA-C1A-NA	-2.10	121.58	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	604	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
28	N	610	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
28	Y	614	CLA	CHA-C1A-NA	-2.10	121.58	126.40
28	B	604	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
28	G	612	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
28	c	508	CLA	O2A-CGA-CBA	2.10	118.50	111.91
28	b	613	CLA	C1D-ND-C4D	-2.10	104.84	106.33
46	Y	605	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
28	C	505	CLA	CHA-C1A-NA	-2.10	121.59	126.40
28	N	610	CLA	O2A-CGA-CBA	2.10	118.49	111.91
30	b	619	BCR	C1-C6-C5	-2.10	119.66	122.61
28	S	611	CLA	O2A-CGA-CBA	2.10	118.49	111.91
28	A	407	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
28	c	503	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
28	b	610	CLA	CHA-C1A-NA	-2.10	121.60	126.40
28	a	405	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
28	b	617	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
46	N	605	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
28	b	608	CLA	CHA-C1A-NA	-2.09	121.60	126.40
28	c	513	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
30	D	404	BCR	C30-C25-C24	2.09	121.70	115.78
30	b	618	BCR	C37-C22-C21	-2.09	119.99	122.92
46	S	606	CHL	C4D-CHA-C1A	2.09	123.80	121.25
30	C	517	BCR	C34-C9-C10	-2.09	119.99	122.92
28	N	604	CLA	O2A-CGA-CBA	2.09	118.47	111.91
30	a	411	BCR	C40-C30-C25	-2.09	106.91	110.30
28	G	610	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
28	S	610	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
28	B	613	CLA	C2D-C1D-ND	2.09	111.64	110.10
28	S	610	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
28	C	511	CLA	C1D-ND-C4D	-2.09	104.85	106.33
28	C	501	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
28	a	405	CLA	OBD-CAD-C3D	-2.09	123.50	128.52
28	N	602	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
29	A	408	PHO	CMC-C2C-C3C	2.09	128.88	124.94
46	S	607	CHL	C1B-CHB-C4A	-2.09	125.98	130.12
28	Y	610	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
28	B	608	CLA	CHA-C1A-NA	-2.09	121.62	126.40
30	a	411	BCR	C4-C5-C6	-2.09	119.70	122.73
47	S	620	LUT	C20-C13-C12	2.09	121.36	118.08
28	d	402	CLA	CMB-C2B-C3B	2.09	128.58	124.68
38	D	409	LHG	C5-O7-C7	-2.09	112.66	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	608	CLA	C1-O2A-CGA	2.09	121.92	116.44
46	Y	606	CHL	C1-O2A-CGA	2.09	121.92	116.44
28	S	613	CLA	CHA-C1A-NA	-2.08	121.62	126.40
28	B	605	CLA	CAA-CBA-CGA	-2.08	107.16	113.25
28	b	615	CLA	C1-O2A-CGA	2.08	121.91	116.44
30	B	619	BCR	C8-C7-C6	-2.08	121.35	127.20
28	b	610	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
28	B	609	CLA	O2A-CGA-CBA	2.08	118.45	111.91
28	c	507	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
28	D	403	CLA	CHA-C1A-NA	-2.08	121.63	126.40
30	c	515	BCR	C36-C18-C17	-2.08	120.00	122.92
28	G	610	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
28	G	602	CLA	C1D-ND-C4D	-2.08	104.86	106.33
29	a	409	PHO	C1-C2-C3	-2.08	122.44	126.04
46	N	609	CHL	CHD-C4C-C3C	2.08	127.90	124.84
28	b	617	CLA	CHA-C1A-NA	-2.08	121.63	126.40
30	a	411	BCR	C35-C13-C12	2.08	121.35	118.08
28	G	613	CLA	C1D-ND-C4D	-2.08	104.86	106.33
41	d	405	PL9	C37-C38-C39	-2.08	122.66	127.66
28	C	507	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
46	Y	607	CHL	C1-C2-C3	-2.08	122.45	126.04
32	a	413	LMG	C8-O7-C10	-2.08	112.68	117.79
28	A	410	CLA	CHA-C1A-NA	-2.08	121.64	126.40
28	Y	602	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
28	A	407	CLA	CHA-C1A-NA	-2.08	121.64	126.40
28	b	604	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
28	b	603	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
28	C	511	CLA	CMB-C2B-C3B	2.07	128.56	124.68
28	b	613	CLA	O2A-CGA-CBA	2.07	118.41	111.91
28	B	613	CLA	CHA-C1A-NA	-2.07	121.65	126.40
28	A	406	CLA	CHA-C1A-NA	-2.07	121.65	126.40
46	N	601	CHL	C4A-NA-C1A	2.07	107.64	106.71
28	b	616	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
28	A	407	CLA	C1D-ND-C4D	-2.07	104.86	106.33
48	G	622	XAT	C20-C13-C14	-2.07	120.02	122.92
29	A	409	PHO	CMC-C2C-C3C	2.07	128.84	124.94
46	N	609	CHL	CHC-C1C-NC	2.07	127.34	124.20
28	C	508	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
28	Y	612	CLA	C1D-ND-C4D	-2.07	104.86	106.33
28	C	504	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
30	B	619	BCR	C38-C26-C27	2.07	117.59	113.62
28	d	402	CLA	CHA-C1A-NA	-2.07	121.66	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	d	405	PL9	O2-C1-C2	-2.07	117.05	121.78
28	Y	611	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
29	A	409	PHO	C1-C2-C3	-2.07	122.47	126.04
41	d	405	PL9	O1-C4-C3	-2.07	118.44	120.72
28	N	613	CLA	CHA-C1A-NA	-2.07	121.67	126.40
28	Y	612	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
28	A	410	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
30	C	516	BCR	C19-C18-C17	2.06	122.11	118.94
28	N	614	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
28	B	617	CLA	O2A-CGA-CBA	2.06	118.38	111.91
28	G	604	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
28	B	611	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
28	b	615	CLA	C1D-ND-C4D	-2.06	104.87	106.33
28	C	509	CLA	O2A-CGA-CBA	2.06	118.38	111.91
47	Y	621	LUT	C16-C1-C6	-2.06	106.95	110.30
28	G	602	CLA	CMB-C2B-C3B	2.06	128.53	124.68
28	a	407	CLA	O2A-CGA-CBA	2.06	118.38	111.91
32	A	413	LMG	O7-C10-O9	-2.06	118.72	123.70
46	S	608	CHL	C1-C2-C3	-2.06	122.48	126.04
28	B	612	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
28	Y	604	CLA	CHA-C1A-NA	-2.06	121.69	126.40
28	C	504	CLA	O2A-CGA-CBA	2.06	118.36	111.91
28	G	604	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
28	a	406	CLA	C1-C2-C3	-2.06	122.49	126.04
28	Y	602	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
47	G	620	LUT	C31-C32-C33	-2.06	120.64	126.42
28	b	603	CLA	CHA-C1A-NA	-2.06	121.69	126.40
41	D	405	PL9	O2-C1-C2	-2.06	117.07	121.78
28	D	402	CLA	O2A-CGA-CBA	2.06	118.36	111.91
35	b	623	DGD	O5D-C1E-C2E	2.06	111.51	108.30
48	G	622	XAT	C18-C5-C6	-2.06	118.82	122.26
28	C	512	CLA	C1D-ND-C4D	-2.06	104.88	106.33
28	G	604	CLA	CHA-C1A-NA	-2.05	121.69	126.40
28	d	402	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
30	c	516	BCR	C31-C1-C6	-2.05	106.97	110.30
28	b	606	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
28	G	611	CLA	CAC-C3C-C4C	2.05	127.47	124.81
28	C	502	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
28	a	410	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
28	b	609	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
28	c	506	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
47	N	621	LUT	C16-C1-C6	-2.05	106.97	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	516	BCR	C19-C18-C17	2.05	122.09	118.94
28	c	508	CLA	C1-O2A-CGA	2.05	121.82	116.44
28	N	610	CLA	C2A-C1A-CHA	2.05	127.44	123.86
28	B	602	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
30	c	514	BCR	C38-C26-C27	2.05	117.55	113.62
38	G	624	LHG	C6-C5-C4	-2.05	106.94	111.79
28	c	506	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
28	C	510	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
28	b	615	CLA	CHA-C1A-NA	-2.05	121.71	126.40
28	B	610	CLA	C1D-ND-C4D	-2.05	104.88	106.33
43	H	101	RRX	C16-C17-C18	-2.05	124.39	127.31
28	A	405	CLA	C1C-C2C-C3C	-2.05	104.81	106.96
28	G	603	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
48	Y	622	XAT	C39-C29-C30	-2.04	120.06	122.92
30	d	404	BCR	C38-C26-C27	2.04	117.54	113.62
28	N	614	CLA	C1-O2A-CGA	2.04	121.81	116.44
47	Y	620	LUT	C15-C35-C34	-2.04	119.29	123.47
28	N	603	CLA	C1D-ND-C4D	-2.04	104.88	106.33
28	C	509	CLA	CHA-C1A-NA	-2.04	121.72	126.40
46	N	607	CHL	C1B-CHB-C4A	-2.04	126.07	130.12
28	B	611	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
28	G	604	CLA	O2A-CGA-CBA	2.04	118.32	111.91
34	B	620	C7Z	C21-C26-C27	2.04	121.56	115.78
28	N	611	CLA	C1D-ND-C4D	-2.04	104.88	106.33
28	S	610	CLA	C1-O2A-CGA	2.04	121.80	116.44
35	C	519	DGD	O1G-C1A-O1A	-2.04	118.44	123.59
28	B	607	CLA	CHA-C1A-NA	-2.04	121.72	126.40
28	c	513	CLA	C1-O2A-CGA	2.04	121.80	116.44
49	Y	623	NEX	C31-C32-C33	2.04	132.15	126.42
28	C	501	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
28	S	617	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
47	N	620	LUT	C15-C35-C34	-2.04	119.29	123.47
28	C	502	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
47	S	621	LUT	C20-C13-C12	2.04	121.29	118.08
28	B	616	CLA	C1D-ND-C4D	-2.04	104.89	106.33
46	Y	605	CHL	C4A-NA-C1A	2.04	107.62	106.71
28	S	603	CLA	C1-O2A-CGA	2.04	121.80	116.44
28	S	603	CLA	C2A-C1A-CHA	2.04	127.42	123.86
28	c	508	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
28	B	606	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
28	b	608	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
28	G	602	CLA	O1D-CGD-CBD	-2.04	120.31	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N	622	XAT	C20-C13-C14	-2.04	120.07	122.92
28	S	611	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
28	S	612	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
28	B	613	CLA	O2A-CGA-CBA	2.04	118.30	111.91
28	c	507	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
28	S	604	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
28	G	604	CLA	C1D-ND-C4D	-2.04	104.89	106.33
28	S	611	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
28	c	507	CLA	C1-C2-C3	-2.03	122.53	126.04
30	d	404	BCR	C33-C5-C6	-2.03	122.25	124.53
28	S	605	CLA	C2D-C1D-ND	2.03	111.60	110.10
30	B	619	BCR	C15-C14-C13	-2.03	124.41	127.31
28	C	503	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
28	S	611	CLA	C2A-C1A-CHA	2.03	127.41	123.86
28	b	613	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
28	N	602	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
28	C	505	CLA	OBD-CAD-C3D	-2.03	123.64	128.52
28	Y	610	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
47	G	620	LUT	C20-C13-C12	2.03	121.28	118.08
28	d	403	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
28	Y	604	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
28	B	605	CLA	C2A-C1A-CHA	2.03	127.41	123.86
32	C	521	LMG	O7-C10-O9	-2.03	118.80	123.70
49	Y	623	NEX	C20-C13-C14	-2.03	120.08	122.92
28	b	612	CLA	C1D-ND-C4D	-2.03	104.89	106.33
47	S	621	LUT	C18-C5-C4	2.03	118.11	114.36
29	A	408	PHO	C1B-NB-C4B	2.03	111.25	107.09
46	N	601	CHL	CHD-C4C-C3C	2.03	127.82	124.84
28	S	617	CLA	C1D-ND-C4D	-2.03	104.90	106.33
41	D	405	PL9	C36-C34-C33	-2.03	117.02	121.12
28	b	609	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
28	B	606	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
34	B	620	C7Z	C24-C25-C26	-2.02	116.33	120.85
28	N	612	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
46	Y	605	CHL	C1B-CHB-C4A	-2.02	126.11	130.12
28	G	610	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
28	S	603	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
28	c	506	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
28	b	605	CLA	CHA-C1A-NA	-2.02	121.76	126.40
34	B	620	C7Z	C1-C6-C7	2.02	121.50	115.78
28	b	609	CLA	C2A-C1A-CHA	2.02	127.40	123.86
28	N	603	CLA	CAA-C2A-C3A	-2.02	107.24	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	402	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
42	F	101	HEM	CMB-C2B-C1B	-2.02	121.96	125.04
28	B	616	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
28	S	613	CLA	O2A-CGA-CBA	2.02	118.25	111.91
28	B	605	CLA	CMB-C2B-C3B	2.02	128.46	124.68
42	f	101	HEM	C3D-C4D-ND	-2.02	107.92	110.17
28	C	508	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
28	d	402	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
28	G	602	CLA	CHA-C1A-NA	-2.02	121.78	126.40
32	C	523	LMG	O7-C10-O9	-2.02	118.83	123.70
28	c	502	CLA	O2A-CGA-CBA	2.02	118.24	111.91
49	Y	623	NEX	C4-C3-C2	2.02	114.67	110.77
28	G	610	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	A	412	SQD	O8-S-C6	-2.02	102.53	105.74
28	N	613	CLA	CMC-C2C-C1C	2.02	128.11	125.04
28	B	612	CLA	CHA-C1A-NA	-2.02	121.78	126.40
46	G	606	CHL	CHA-C1A-NA	-2.02	121.78	126.40
28	S	602	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
28	Y	610	CLA	CHA-C1A-NA	-2.01	121.78	126.40
28	S	612	CLA	CMA-C3A-C4A	2.01	117.19	111.77
32	C	523	LMG	C8-O7-C10	-2.01	112.83	117.79
46	S	608	CHL	C4D-CHA-C1A	2.01	123.70	121.25
28	Y	610	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
46	N	606	CHL	C4D-CHA-C1A	2.01	123.70	121.25
28	S	609	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
28	a	405	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
28	S	617	CLA	C1-O2A-CGA	2.01	121.72	116.44
41	D	405	PL9	C37-C38-C39	-2.01	122.82	127.66
28	B	616	CLA	CMA-C3A-C4A	2.01	117.18	111.77
28	Y	602	CLA	CHA-C1A-NA	-2.01	121.79	126.40
28	A	407	CLA	C1-O2A-CGA	2.01	121.72	116.44
30	a	411	BCR	C34-C9-C10	-2.01	120.11	122.92
47	Y	621	LUT	C35-C15-C14	-2.01	119.36	123.47
28	b	604	CLA	CMB-C2B-C3B	2.01	128.44	124.68
28	a	406	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
28	Y	608	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
28	Y	603	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
28	C	503	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
28	B	606	CLA	CHA-C1A-NA	-2.01	121.80	126.40
28	d	402	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
28	A	406	CLA	C2A-C1A-CHA	2.01	127.37	123.86
28	a	410	CLA	C1-C2-C3	-2.01	122.58	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	609	CLA	CBC-CAC-C3C	-2.00	106.91	112.43
28	G	610	CLA	CHA-C1A-NA	-2.00	121.81	126.40
30	D	404	BCR	C38-C26-C27	2.00	117.47	113.62
28	b	602	CLA	O2A-CGA-CBA	2.00	118.19	111.91
28	S	613	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
28	C	502	CLA	C1-O2A-CGA	2.00	121.70	116.44
28	b	613	CLA	CMA-C3A-C4A	2.00	117.16	111.77
28	G	613	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
28	a	405	CLA	CHA-C1A-NA	-2.00	121.81	126.40
28	N	604	CLA	C1D-ND-C4D	-2.00	104.91	106.33
28	S	610	CLA	CMA-C3A-C4A	2.00	117.15	111.77
34	B	620	C7Z	C15-C35-C34	-2.00	119.37	123.47
28	C	508	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
28	b	607	CLA	CMA-C3A-C4A	2.00	117.15	111.77
30	b	619	BCR	C36-C18-C17	-2.00	120.12	122.92
28	S	612	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
28	Y	604	CLA	O1D-CGD-CBD	-2.00	120.39	124.48

All (194) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	A	405	CLA	ND
28	A	406	CLA	ND
28	A	407	CLA	ND
28	A	410	CLA	ND
28	B	602	CLA	ND
28	B	603	CLA	ND
28	B	604	CLA	ND
28	B	605	CLA	ND
28	B	606	CLA	ND
28	B	607	CLA	ND
28	B	608	CLA	ND
28	B	609	CLA	ND
28	B	610	CLA	ND
28	B	611	CLA	ND
28	B	612	CLA	ND
28	B	613	CLA	ND
28	B	614	CLA	ND
28	B	615	CLA	ND
28	B	616	CLA	ND
28	B	617	CLA	ND
28	C	501	CLA	ND

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Mol	Chain	Res	Type	Atom
28	C	502	CLA	ND
28	C	503	CLA	ND
28	C	504	CLA	ND
28	C	505	CLA	ND
28	C	506	CLA	ND
28	C	507	CLA	ND
28	C	508	CLA	ND
28	C	509	CLA	ND
28	C	510	CLA	ND
28	C	511	CLA	ND
28	C	512	CLA	ND
28	C	513	CLA	ND
28	D	402	CLA	ND
28	D	403	CLA	ND
28	N	602	CLA	ND
28	N	603	CLA	ND
28	N	604	CLA	ND
28	N	610	CLA	ND
28	N	611	CLA	ND
28	N	612	CLA	ND
28	N	613	CLA	ND
28	N	614	CLA	ND
28	G	602	CLA	ND
28	G	603	CLA	ND
28	G	604	CLA	ND
28	G	610	CLA	ND
28	G	611	CLA	ND
28	G	612	CLA	ND
28	G	613	CLA	ND
28	G	614	CLA	ND
28	S	602	CLA	ND
28	S	603	CLA	ND
28	S	604	CLA	ND
28	S	605	CLA	ND
28	S	609	CLA	ND
28	S	610	CLA	ND
28	S	611	CLA	ND
28	S	612	CLA	ND
28	S	613	CLA	ND
28	S	614	CLA	ND
28	S	617	CLA	ND
28	Y	602	CLA	ND

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Mol	Chain	Res	Type	Atom
28	Y	603	CLA	ND
28	Y	604	CLA	ND
28	Y	608	CLA	ND
28	Y	610	CLA	ND
28	Y	611	CLA	ND
28	Y	612	CLA	ND
28	Y	613	CLA	ND
28	Y	614	CLA	ND
28	a	405	CLA	ND
28	a	406	CLA	ND
28	a	407	CLA	ND
28	a	410	CLA	ND
28	b	602	CLA	ND
28	b	603	CLA	ND
28	b	604	CLA	ND
28	b	605	CLA	ND
28	b	606	CLA	ND
28	b	607	CLA	ND
28	b	608	CLA	ND
28	b	609	CLA	ND
28	b	610	CLA	ND
28	b	611	CLA	ND
28	b	612	CLA	ND
28	b	613	CLA	ND
28	b	614	CLA	ND
28	b	615	CLA	ND
28	b	616	CLA	ND
28	b	617	CLA	ND
28	c	501	CLA	ND
28	c	502	CLA	ND
28	c	503	CLA	ND
28	c	504	CLA	ND
28	c	505	CLA	ND
28	c	506	CLA	ND
28	c	507	CLA	ND
28	c	508	CLA	ND
28	c	509	CLA	ND
28	c	510	CLA	ND
28	c	511	CLA	ND
28	c	512	CLA	ND
28	c	513	CLA	ND
28	d	402	CLA	ND

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Mol	Chain	Res	Type	Atom
28	d	403	CLA	ND
34	B	620	C7Z	C3
34	b	620	C7Z	C3
39	C	527	LMK	C3
39	C	527	LMK	C8
39	c	527	LMK	C3
39	c	527	LMK	C8
43	H	101	RRX	C28
43	h	101	RRX	C28
46	N	601	CHL	NC
46	N	601	CHL	NA
46	N	601	CHL	C8
46	N	601	CHL	ND
46	N	605	CHL	NC
46	N	605	CHL	NA
46	N	605	CHL	C8
46	N	605	CHL	ND
46	N	606	CHL	NC
46	N	606	CHL	NA
46	N	606	CHL	C8
46	N	606	CHL	ND
46	N	607	CHL	NC
46	N	607	CHL	NA
46	N	607	CHL	C8
46	N	607	CHL	ND
46	N	608	CHL	NC
46	N	608	CHL	NA
46	N	608	CHL	ND
46	N	609	CHL	NC
46	N	609	CHL	NA
46	N	609	CHL	C8
46	N	609	CHL	ND
46	G	601	CHL	NC
46	G	601	CHL	NA
46	G	601	CHL	C8
46	G	601	CHL	ND
46	G	605	CHL	NC
46	G	605	CHL	NA
46	G	605	CHL	C3A
46	G	605	CHL	ND
46	G	606	CHL	NC
46	G	606	CHL	NA

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Mol	Chain	Res	Type	Atom
46	G	606	CHL	ND
46	G	607	CHL	NC
46	G	607	CHL	NA
46	G	607	CHL	C8
46	G	607	CHL	ND
46	G	608	CHL	NC
46	G	608	CHL	NA
46	G	608	CHL	ND
46	G	609	CHL	NC
46	G	609	CHL	NA
46	G	609	CHL	C8
46	G	609	CHL	ND
46	S	601	CHL	NC
46	S	601	CHL	NA
46	S	601	CHL	ND
46	S	606	CHL	NC
46	S	606	CHL	NA
46	S	606	CHL	ND
46	S	607	CHL	NC
46	S	607	CHL	NA
46	S	607	CHL	ND
46	S	608	CHL	NC
46	S	608	CHL	NA
46	S	608	CHL	C8
46	S	608	CHL	ND
46	Y	601	CHL	NC
46	Y	601	CHL	NA
46	Y	601	CHL	C8
46	Y	601	CHL	ND
46	Y	605	CHL	NC
46	Y	605	CHL	NA
46	Y	605	CHL	ND
46	Y	606	CHL	NC
46	Y	606	CHL	NA
46	Y	606	CHL	C8
46	Y	606	CHL	ND
46	Y	607	CHL	NC
46	Y	607	CHL	NA
46	Y	607	CHL	C8
46	Y	607	CHL	ND
46	Y	609	CHL	NC
46	Y	609	CHL	NA

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Mol	Chain	Res	Type	Atom
46	Y	609	CHL	C8
46	Y	609	CHL	ND
48	N	622	XAT	C6
48	G	622	XAT	C26
48	G	622	XAT	C6

All (3369) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	405	CLA	C1A-C2A-CAA-CBA
28	A	405	CLA	C3A-C2A-CAA-CBA
28	A	405	CLA	CBD-CGD-O2D-CED
28	A	406	CLA	C1A-C2A-CAA-CBA
28	A	406	CLA	C3A-C2A-CAA-CBA
28	A	406	CLA	CHA-CBD-CGD-O1D
28	A	406	CLA	CHA-CBD-CGD-O2D
28	A	407	CLA	C2-C1-O2A-CGA
28	A	407	CLA	CHA-CBD-CGD-O1D
28	A	407	CLA	CHA-CBD-CGD-O2D
28	B	602	CLA	C3A-C2A-CAA-CBA
28	B	602	CLA	CHA-CBD-CGD-O1D
28	B	602	CLA	CHA-CBD-CGD-O2D
28	B	602	CLA	CAD-CBD-CGD-O1D
28	B	603	CLA	CHA-CBD-CGD-O1D
28	B	603	CLA	CHA-CBD-CGD-O2D
28	B	603	CLA	CBD-CGD-O2D-CED
28	B	603	CLA	C2-C3-C5-C6
28	B	603	CLA	C4-C3-C5-C6
28	B	604	CLA	C2-C3-C5-C6
28	B	604	CLA	C4-C3-C5-C6
28	B	604	CLA	C14-C13-C15-C16
28	B	605	CLA	C2-C3-C5-C6
28	B	605	CLA	C4-C3-C5-C6
28	B	607	CLA	CBD-CGD-O2D-CED
28	B	608	CLA	C1A-C2A-CAA-CBA
28	B	608	CLA	C3A-C2A-CAA-CBA
28	B	608	CLA	CHA-CBD-CGD-O1D
28	B	608	CLA	CHA-CBD-CGD-O2D
28	B	608	CLA	CAD-CBD-CGD-O1D
28	B	608	CLA	C2-C3-C5-C6
28	B	608	CLA	C4-C3-C5-C6
28	B	609	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	B	610	CLA	C1A-C2A-CAA-CBA
28	B	610	CLA	C3A-C2A-CAA-CBA
28	B	610	CLA	CHA-CBD-CGD-O1D
28	B	610	CLA	CHA-CBD-CGD-O2D
28	B	610	CLA	CAD-CBD-CGD-O1D
28	B	610	CLA	CAD-CBD-CGD-O2D
28	B	612	CLA	CHA-CBD-CGD-O1D
28	B	612	CLA	CHA-CBD-CGD-O2D
28	B	612	CLA	CBD-CGD-O2D-CED
28	B	613	CLA	C1A-C2A-CAA-CBA
28	B	613	CLA	C2-C1-O2A-CGA
28	B	615	CLA	CBD-CGD-O2D-CED
28	B	616	CLA	CHA-CBD-CGD-O1D
28	B	616	CLA	CHA-CBD-CGD-O2D
28	B	617	CLA	CHA-CBD-CGD-O1D
28	B	617	CLA	CHA-CBD-CGD-O2D
28	C	502	CLA	CHA-CBD-CGD-O1D
28	C	502	CLA	CHA-CBD-CGD-O2D
28	C	502	CLA	CAD-CBD-CGD-O1D
28	C	502	CLA	CBD-CGD-O2D-CED
28	C	503	CLA	CBD-CGD-O2D-CED
28	C	503	CLA	C2-C3-C5-C6
28	C	503	CLA	C4-C3-C5-C6
28	C	504	CLA	CBD-CGD-O2D-CED
28	C	504	CLA	C2-C3-C5-C6
28	C	504	CLA	C4-C3-C5-C6
28	C	505	CLA	CHA-CBD-CGD-O1D
28	C	505	CLA	CHA-CBD-CGD-O2D
28	C	505	CLA	CAD-CBD-CGD-O1D
28	C	505	CLA	CAD-CBD-CGD-O2D
28	C	506	CLA	C2-C1-O2A-CGA
28	C	506	CLA	CBD-CGD-O2D-CED
28	C	508	CLA	CHA-CBD-CGD-O1D
28	C	508	CLA	CHA-CBD-CGD-O2D
28	C	509	CLA	C6-C7-C8-C9
28	C	511	CLA	CBD-CGD-O2D-CED
28	C	512	CLA	CBA-CGA-O2A-C1
28	C	512	CLA	CHA-CBD-CGD-O1D
28	C	512	CLA	CHA-CBD-CGD-O2D
28	C	512	CLA	CAD-CBD-CGD-O1D
28	C	513	CLA	C1A-C2A-CAA-CBA
28	C	513	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	D	402	CLA	C3A-C2A-CAA-CBA
28	D	402	CLA	C2-C3-C5-C6
28	D	402	CLA	C4-C3-C5-C6
28	D	403	CLA	O1A-CGA-O2A-C1
28	D	403	CLA	CBD-CGD-O2D-CED
28	N	604	CLA	C1A-C2A-CAA-CBA
28	N	604	CLA	C3A-C2A-CAA-CBA
28	N	610	CLA	C1A-C2A-CAA-CBA
28	N	610	CLA	C3A-C2A-CAA-CBA
28	N	610	CLA	C2-C3-C5-C6
28	N	610	CLA	C4-C3-C5-C6
28	N	611	CLA	CHA-CBD-CGD-O1D
28	N	611	CLA	CHA-CBD-CGD-O2D
28	N	612	CLA	CBD-CGD-O2D-CED
28	N	613	CLA	C1A-C2A-CAA-CBA
28	N	613	CLA	CHA-CBD-CGD-O1D
28	N	613	CLA	CHA-CBD-CGD-O2D
28	N	614	CLA	C1A-C2A-CAA-CBA
28	G	602	CLA	C1A-C2A-CAA-CBA
28	G	602	CLA	C3A-C2A-CAA-CBA
28	G	603	CLA	CBD-CGD-O2D-CED
28	G	610	CLA	CBD-CGD-O2D-CED
28	G	614	CLA	CBD-CGD-O2D-CED
28	S	602	CLA	C2-C1-O2A-CGA
28	S	602	CLA	CHA-CBD-CGD-O1D
28	S	602	CLA	CHA-CBD-CGD-O2D
28	S	603	CLA	C1A-C2A-CAA-CBA
28	S	603	CLA	C3A-C2A-CAA-CBA
28	S	603	CLA	CHA-CBD-CGD-O1D
28	S	603	CLA	CHA-CBD-CGD-O2D
28	S	604	CLA	CBA-CGA-O2A-C1
28	S	604	CLA	O1A-CGA-O2A-C1
28	S	604	CLA	CBD-CGD-O2D-CED
28	S	605	CLA	C1A-C2A-CAA-CBA
28	S	605	CLA	CHA-CBD-CGD-O1D
28	S	605	CLA	CHA-CBD-CGD-O2D
28	S	609	CLA	CBD-CGD-O2D-CED
28	S	610	CLA	C1A-C2A-CAA-CBA
28	S	610	CLA	C3A-C2A-CAA-CBA
28	S	610	CLA	CBD-CGD-O2D-CED
28	S	611	CLA	C1A-C2A-CAA-CBA
28	S	611	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	S	611	CLA	CAD-CBD-CGD-O2D
28	S	611	CLA	CBD-CGD-O2D-CED
28	S	612	CLA	CBD-CGD-O2D-CED
28	S	613	CLA	CHA-CBD-CGD-O1D
28	S	613	CLA	CHA-CBD-CGD-O2D
28	S	614	CLA	CBD-CGD-O2D-CED
28	Y	604	CLA	CBD-CGD-O2D-CED
28	Y	608	CLA	C2-C1-O2A-CGA
28	Y	610	CLA	CBD-CGD-O2D-CED
28	Y	611	CLA	CHA-CBD-CGD-O1D
28	Y	611	CLA	CHA-CBD-CGD-O2D
28	Y	614	CLA	CBD-CGD-O2D-CED
28	a	405	CLA	C1A-C2A-CAA-CBA
28	a	405	CLA	C3A-C2A-CAA-CBA
28	a	405	CLA	CBD-CGD-O2D-CED
28	a	406	CLA	C3A-C2A-CAA-CBA
28	a	406	CLA	C2-C1-O2A-CGA
28	a	406	CLA	CHA-CBD-CGD-O1D
28	a	406	CLA	CHA-CBD-CGD-O2D
28	b	602	CLA	CHA-CBD-CGD-O1D
28	b	602	CLA	CHA-CBD-CGD-O2D
28	b	603	CLA	CHA-CBD-CGD-O1D
28	b	603	CLA	CHA-CBD-CGD-O2D
28	b	603	CLA	CBD-CGD-O2D-CED
28	b	604	CLA	CBD-CGD-O2D-CED
28	b	606	CLA	CBD-CGD-O2D-CED
28	b	606	CLA	C4-C3-C5-C6
28	b	607	CLA	C1A-C2A-CAA-CBA
28	b	607	CLA	CHA-CBD-CGD-O1D
28	b	607	CLA	CHA-CBD-CGD-O2D
28	b	607	CLA	CBD-CGD-O2D-CED
28	b	608	CLA	C1A-C2A-CAA-CBA
28	b	608	CLA	C3A-C2A-CAA-CBA
28	b	608	CLA	CHA-CBD-CGD-O1D
28	b	608	CLA	CHA-CBD-CGD-O2D
28	b	608	CLA	CAD-CBD-CGD-O1D
28	b	608	CLA	C2-C3-C5-C6
28	b	608	CLA	C4-C3-C5-C6
28	b	609	CLA	C1A-C2A-CAA-CBA
28	b	609	CLA	C3A-C2A-CAA-CBA
28	b	609	CLA	CHA-CBD-CGD-O1D
28	b	609	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	b	610	CLA	C1A-C2A-CAA-CBA
28	b	610	CLA	C3A-C2A-CAA-CBA
28	b	610	CLA	CAD-CBD-CGD-O1D
28	b	610	CLA	CAD-CBD-CGD-O2D
28	b	611	CLA	CBD-CGD-O2D-CED
28	b	613	CLA	C2-C1-O2A-CGA
28	b	614	CLA	CHA-CBD-CGD-O1D
28	b	614	CLA	CHA-CBD-CGD-O2D
28	b	616	CLA	CHA-CBD-CGD-O1D
28	b	616	CLA	CHA-CBD-CGD-O2D
28	c	501	CLA	CHA-CBD-CGD-O1D
28	c	501	CLA	CHA-CBD-CGD-O2D
28	c	501	CLA	CAD-CBD-CGD-O1D
28	c	501	CLA	CBD-CGD-O2D-CED
28	c	502	CLA	CAD-CBD-CGD-O1D
28	c	502	CLA	CAD-CBD-CGD-O2D
28	c	502	CLA	CBD-CGD-O2D-CED
28	c	503	CLA	C2-C3-C5-C6
28	c	503	CLA	C4-C3-C5-C6
28	c	504	CLA	C1A-C2A-CAA-CBA
28	c	504	CLA	C3A-C2A-CAA-CBA
28	c	504	CLA	C6-C7-C8-C9
28	c	506	CLA	C2-C1-O2A-CGA
28	c	506	CLA	CBD-CGD-O2D-CED
28	c	508	CLA	CHA-CBD-CGD-O1D
28	c	508	CLA	CHA-CBD-CGD-O2D
28	c	509	CLA	C2-C1-O2A-CGA
28	c	509	CLA	CBD-CGD-O2D-CED
28	c	510	CLA	CHA-CBD-CGD-O1D
28	c	510	CLA	CHA-CBD-CGD-O2D
28	c	510	CLA	CBD-CGD-O2D-CED
28	c	511	CLA	C1A-C2A-CAA-CBA
28	c	511	CLA	CHA-CBD-CGD-O1D
28	c	511	CLA	CHA-CBD-CGD-O2D
28	c	512	CLA	CBA-CGA-O2A-C1
28	c	512	CLA	O1A-CGA-O2A-C1
28	c	512	CLA	CHA-CBD-CGD-O1D
28	c	512	CLA	CHA-CBD-CGD-O2D
28	c	512	CLA	CAD-CBD-CGD-O1D
28	c	513	CLA	C1A-C2A-CAA-CBA
28	d	402	CLA	C2-C1-O2A-CGA
28	d	402	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	d	402	CLA	CHA-CBD-CGD-O2D
28	d	402	CLA	CBD-CGD-O2D-CED
28	d	403	CLA	CBA-CGA-O2A-C1
28	d	403	CLA	O1A-CGA-O2A-C1
28	d	403	CLA	C2-C3-C5-C6
28	d	403	CLA	C4-C3-C5-C6
29	A	409	PHO	C3A-C2A-CAA-CBA
29	a	409	PHO	C3A-C2A-CAA-CBA
30	A	411	BCR	C7-C8-C9-C10
30	A	411	BCR	C7-C8-C9-C34
30	A	411	BCR	C11-C10-C9-C8
30	A	411	BCR	C11-C10-C9-C34
30	A	411	BCR	C10-C11-C12-C13
30	A	411	BCR	C17-C18-C19-C20
30	A	411	BCR	C36-C18-C19-C20
30	B	618	BCR	C11-C10-C9-C8
30	B	618	BCR	C11-C10-C9-C34
30	B	618	BCR	C10-C11-C12-C13
30	B	618	BCR	C17-C18-C19-C20
30	B	618	BCR	C36-C18-C19-C20
30	B	619	BCR	C11-C10-C9-C8
30	B	619	BCR	C11-C10-C9-C34
30	C	514	BCR	C11-C10-C9-C8
30	C	514	BCR	C11-C10-C9-C34
30	C	514	BCR	C9-C10-C11-C12
30	C	514	BCR	C10-C11-C12-C13
30	C	514	BCR	C13-C14-C15-C16
30	C	514	BCR	C36-C18-C19-C20
30	C	514	BCR	C37-C22-C23-C24
30	C	515	BCR	C11-C10-C9-C8
30	C	515	BCR	C11-C10-C9-C34
30	C	515	BCR	C10-C11-C12-C13
30	C	515	BCR	C17-C18-C19-C20
30	C	515	BCR	C36-C18-C19-C20
30	C	515	BCR	C19-C20-C21-C22
30	C	516	BCR	C1-C6-C7-C8
30	C	516	BCR	C5-C6-C7-C8
30	C	516	BCR	C7-C8-C9-C10
30	C	516	BCR	C7-C8-C9-C34
30	C	516	BCR	C11-C10-C9-C8
30	C	516	BCR	C11-C10-C9-C34
30	C	516	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	C	516	BCR	C23-C24-C25-C30
30	C	517	BCR	C11-C10-C9-C8
30	C	517	BCR	C11-C10-C9-C34
30	C	517	BCR	C10-C11-C12-C13
30	C	517	BCR	C17-C18-C19-C20
30	C	517	BCR	C36-C18-C19-C20
30	D	404	BCR	C11-C10-C9-C8
30	D	404	BCR	C11-C10-C9-C34
30	D	404	BCR	C10-C11-C12-C13
30	D	404	BCR	C17-C18-C19-C20
30	D	404	BCR	C36-C18-C19-C20
30	D	404	BCR	C21-C22-C23-C24
30	D	404	BCR	C37-C22-C23-C24
30	D	404	BCR	C23-C24-C25-C26
30	D	404	BCR	C23-C24-C25-C30
30	a	411	BCR	C11-C10-C9-C8
30	a	411	BCR	C11-C10-C9-C34
30	a	411	BCR	C17-C18-C19-C20
30	a	411	BCR	C36-C18-C19-C20
30	b	618	BCR	C11-C10-C9-C8
30	b	618	BCR	C11-C10-C9-C34
30	b	618	BCR	C10-C11-C12-C13
30	b	619	BCR	C7-C8-C9-C10
30	b	619	BCR	C7-C8-C9-C34
30	b	619	BCR	C11-C10-C9-C8
30	b	619	BCR	C11-C10-C9-C34
30	b	619	BCR	C10-C11-C12-C13
30	b	619	BCR	C36-C18-C19-C20
30	b	619	BCR	C23-C24-C25-C30
30	c	514	BCR	C11-C10-C9-C8
30	c	514	BCR	C11-C10-C9-C34
30	c	514	BCR	C9-C10-C11-C12
30	c	514	BCR	C10-C11-C12-C13
30	c	514	BCR	C17-C18-C19-C20
30	c	514	BCR	C36-C18-C19-C20
30	c	515	BCR	C7-C8-C9-C34
30	c	515	BCR	C11-C10-C9-C8
30	c	515	BCR	C11-C10-C9-C34
30	c	516	BCR	C7-C8-C9-C10
30	c	516	BCR	C7-C8-C9-C34
30	c	516	BCR	C9-C10-C11-C12
30	c	516	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	c	516	BCR	C21-C22-C23-C24
30	c	516	BCR	C37-C22-C23-C24
30	c	517	BCR	C11-C10-C9-C8
30	c	517	BCR	C11-C10-C9-C34
30	c	517	BCR	C10-C11-C12-C13
30	d	404	BCR	C11-C10-C9-C8
30	d	404	BCR	C11-C10-C9-C34
30	d	404	BCR	C10-C11-C12-C13
30	d	404	BCR	C36-C18-C19-C20
30	d	404	BCR	C23-C24-C25-C26
30	d	404	BCR	C23-C24-C25-C30
31	B	621	SQD	C2-C1-O6-C44
31	B	621	SQD	O5-C1-O6-C44
31	B	621	SQD	O5-C5-C6-S
31	B	626	SQD	O47-C45-C46-O48
31	B	626	SQD	C5-C6-S-O7
31	B	626	SQD	C5-C6-S-O8
31	B	626	SQD	C5-C6-S-O9
31	C	526	SQD	O5-C5-C6-S
31	C	526	SQD	C5-C6-S-O7
31	C	526	SQD	C5-C6-S-O8
31	C	526	SQD	C5-C6-S-O9
31	M	101	SQD	O5-C5-C6-S
31	a	412	SQD	O47-C45-C46-O48
31	a	412	SQD	O5-C5-C6-S
31	b	621	SQD	C2-C1-O6-C44
31	b	621	SQD	O5-C1-O6-C44
31	b	621	SQD	O5-C5-C6-S
31	b	626	SQD	C2-C1-O6-C44
31	b	626	SQD	O5-C1-O6-C44
31	b	626	SQD	C5-C6-S-O7
31	b	626	SQD	C5-C6-S-O8
31	b	626	SQD	C5-C6-S-O9
31	c	526	SQD	O5-C5-C6-S
31	m	101	SQD	C2-C1-O6-C44
31	m	101	SQD	O5-C1-O6-C44
31	m	101	SQD	O5-C5-C6-S
31	m	101	SQD	C5-C6-S-O7
31	m	101	SQD	C5-C6-S-O8
31	m	101	SQD	C5-C6-S-O9
32	A	413	LMG	C2-C1-O1-C7
32	A	413	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
32	B	622	LMG	O6-C1-O1-C7
32	B	622	LMG	O9-C10-O7-C8
32	B	622	LMG	C11-C10-O7-C8
32	C	523	LMG	C2-C1-O1-C7
32	C	523	LMG	O6-C1-O1-C7
32	W	201	LMG	O6-C1-O1-C7
32	W	201	LMG	C7-C8-O7-C10
32	W	201	LMG	C11-C10-O7-C8
32	W	201	LMG	O10-C28-O8-C9
32	b	622	LMG	O9-C10-O7-C8
32	b	622	LMG	C11-C10-O7-C8
32	c	523	LMG	C11-C10-O7-C8
33	A	414	SPH	C1-C2-C3-O3
33	Y	625	SPH	O1-C1-C2-N2
33	Y	625	SPH	O1-C1-C2-C3
33	Y	625	SPH	C2-C3-C4-C5
33	Y	625	SPH	O3-C3-C4-C5
33	a	414	SPH	O1-C1-C2-N2
33	a	414	SPH	O1-C1-C2-C3
33	a	414	SPH	C1-C2-C3-O3
33	a	414	SPH	C1-C2-C3-C4
33	a	414	SPH	N2-C2-C3-O3
33	a	414	SPH	N2-C2-C3-C4
34	B	620	C7Z	C11-C12-C13-C20
34	B	620	C7Z	C11-C12-C13-C14
34	B	620	C7Z	C27-C28-C29-C30
34	B	620	C7Z	C27-C28-C29-C39
34	b	620	C7Z	C21-C26-C27-C28
34	b	620	C7Z	C11-C12-C13-C20
34	b	620	C7Z	C11-C12-C13-C14
34	b	620	C7Z	C31-C32-C33-C40
34	b	620	C7Z	C27-C28-C29-C30
34	b	620	C7Z	C27-C28-C29-C39
35	B	623	DGD	O1B-C1B-O2G-C2G
35	B	623	DGD	O6D-C1D-O3G-C3G
35	B	623	DGD	C2E-C1E-O5D-C6D
35	B	623	DGD	O6E-C1E-O5D-C6D
35	b	623	DGD	O1B-C1B-O2G-C2G
35	b	623	DGD	O6D-C1D-O3G-C3G
35	c	518	DGD	C2E-C1E-O5D-C6D
35	c	518	DGD	O6E-C1E-O5D-C6D
36	B	624	3PH	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
36	B	624	3PH	C1-O11-P-O14
36	B	624	3PH	C1-O11-P-O12
36	T	101	3PH	C1-O11-P-O13
36	T	101	3PH	C1-O11-P-O14
36	S	626	3PH	O22-C21-O21-C2
36	b	624	3PH	O21-C2-C3-O31
36	t	101	3PH	O22-C21-O21-C2
36	t	101	3PH	C22-C21-O21-C2
37	B	625	DGA	CB2-CB1-OG2-CG2
37	B	625	DGA	OB1-CB1-OG2-CG2
37	B	625	DGA	CG1-CG2-CG3-OXT
37	B	625	DGA	OG2-CG2-CG3-OXT
37	J	101	DGA	CG1-CG2-CG3-OXT
37	J	101	DGA	OG2-CG2-CG3-OXT
37	b	625	DGA	CB2-CB1-OG2-CG2
37	b	625	DGA	OB1-CB1-OG2-CG2
37	b	625	DGA	CG1-CG2-CG3-OXT
37	b	625	DGA	OG2-CG2-CG3-OXT
38	C	525	LHG	O1-C1-C2-O2
38	C	525	LHG	C3-O3-P-O6
38	C	525	LHG	C4-O6-P-O4
38	D	408	LHG	O1-C1-C2-C3
38	D	408	LHG	C3-O3-P-O5
38	D	408	LHG	C4-O6-P-O3
38	D	408	LHG	C4-O6-P-O4
38	D	408	LHG	C4-O6-P-O5
38	D	409	LHG	C4-O6-P-O4
38	D	410	LHG	C3-O3-P-O4
38	D	410	LHG	C3-O3-P-O5
38	D	410	LHG	C4-O6-P-O5
38	D	410	LHG	O7-C5-C6-O8
38	L	101	LHG	O1-C1-C2-O2
38	L	101	LHG	C3-O3-P-O4
38	L	101	LHG	C3-O3-P-O5
38	L	101	LHG	C3-O3-P-O6
38	L	101	LHG	O9-C7-O7-C5
38	L	101	LHG	C8-C7-O7-C5
38	N	624	LHG	O1-C1-C2-C3
38	N	624	LHG	C4-O6-P-O4
38	N	624	LHG	O7-C5-C6-O8
38	G	624	LHG	C4-O6-P-O4
38	G	624	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
38	S	624	LHG	O1-C1-C2-C3
38	S	624	LHG	O2-C2-C3-O3
38	S	624	LHG	C3-O3-P-O5
38	S	624	LHG	C4-O6-P-O3
38	S	624	LHG	C4-O6-P-O4
38	S	624	LHG	C4-O6-P-O5
38	S	624	LHG	C8-C7-O7-C5
38	Y	624	LHG	C1-C2-C3-O3
38	Y	624	LHG	C4-O6-P-O4
38	Y	624	LHG	C4-O6-P-O5
38	c	525	LHG	C1-C2-C3-O3
38	c	525	LHG	C3-O3-P-O5
38	c	525	LHG	C3-O3-P-O6
38	c	525	LHG	C4-O6-P-O4
38	d	408	LHG	O1-C1-C2-C3
38	d	408	LHG	C3-O3-P-O4
38	d	408	LHG	C4-O6-P-O3
38	d	408	LHG	C4-O6-P-O4
38	d	408	LHG	C4-O6-P-O5
38	d	409	LHG	C3-O3-P-O5
38	d	410	LHG	O1-C1-C2-C3
38	d	410	LHG	C3-O3-P-O5
38	d	410	LHG	C4-O6-P-O3
38	d	410	LHG	C4-O6-P-O4
38	d	410	LHG	C4-O6-P-O5
38	l	101	LHG	O1-C1-C2-C3
38	l	101	LHG	C3-O3-P-O4
38	l	101	LHG	C3-O3-P-O5
38	l	101	LHG	C3-O3-P-O6
38	l	101	LHG	O9-C7-O7-C5
38	l	101	LHG	C8-C7-O7-C5
39	C	527	LMK	O9-C10-O7-C8
39	C	527	LMK	C1-C2-C3-C4
39	C	527	LMK	C1-C2-C3-N4
39	C	527	LMK	C2-C3-N4-C5
39	C	527	LMK	C2-C3-N4-C6
39	C	527	LMK	C2-C3-N4-C46
39	c	527	LMK	O1-C7-C8-O7
39	c	527	LMK	O9-C10-C11-C12
39	c	527	LMK	O10-C28-O8-C9
41	d	405	PL9	C12-C13-C14-C16
41	d	405	PL9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
41	d	405	PL9	C24-C26-C27-C28
41	d	405	PL9	C27-C28-C29-C31
41	d	405	PL9	C32-C33-C34-C36
41	d	405	PL9	C37-C38-C39-C40
43	H	101	RRX	C23-C24-C25-C26
43	h	101	RRX	C23-C24-C25-C26
43	h	101	RRX	C36-C18-C19-C20
43	h	101	RRX	C17-C18-C19-C20
43	h	101	RRX	C5-C6-C7-C8
44	I	101	GOL	C1-C2-C3-O3
45	I	102	4RF	O18-C19-C20-O21
45	I	102	4RF	C24-C22-O21-C20
45	K	101	4RF	O21-C20-C39-O40
45	i	101	4RF	C24-C22-O21-C20
46	N	606	CHL	C2-C3-C5-C6
46	G	601	CHL	CHA-CBD-CGD-O1D
46	G	601	CHL	CHA-CBD-CGD-O2D
46	G	605	CHL	C1A-C2A-CAA-CBA
46	G	605	CHL	C3A-C2A-CAA-CBA
46	G	605	CHL	CHA-CBD-CGD-O1D
46	G	605	CHL	CHA-CBD-CGD-O2D
46	G	607	CHL	C1A-C2A-CAA-CBA
46	G	609	CHL	CHA-CBD-CGD-O1D
46	G	609	CHL	CHA-CBD-CGD-O2D
46	G	609	CHL	C2-C3-C5-C6
46	G	609	CHL	C4-C3-C5-C6
46	Y	601	CHL	CHA-CBD-CGD-O1D
46	Y	601	CHL	CHA-CBD-CGD-O2D
47	N	620	LUT	C1-C6-C7-C8
47	N	621	LUT	C21-C26-C27-C28
47	G	620	LUT	C27-C28-C29-C30
47	G	620	LUT	C27-C28-C29-C39
47	G	621	LUT	C21-C26-C27-C28
47	S	620	LUT	C25-C26-C27-C28
47	Y	621	LUT	C21-C26-C27-C28
50	S	625	LPX	C3-C4-C5-O6
50	S	625	LPX	O1-C3-C4-C5
50	S	625	LPX	C1-O2-P1-O3
50	S	625	LPX	C1-O2-P1-O4
51	Y	626	PTY	N1-C2-C3-O11
51	Y	627	PTY	C11-C8-O7-C6
28	G	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	S	613	CLA	O1D-CGD-O2D-CED
28	b	614	CLA	O1D-CGD-O2D-CED
28	N	613	CLA	O1D-CGD-O2D-CED
28	Y	608	CLA	O1D-CGD-O2D-CED
28	Y	613	CLA	O1D-CGD-O2D-CED
28	a	405	CLA	O1D-CGD-O2D-CED
28	b	608	CLA	O1D-CGD-O2D-CED
28	A	410	CLA	CBD-CGD-O2D-CED
28	B	604	CLA	CBD-CGD-O2D-CED
28	B	606	CLA	CBD-CGD-O2D-CED
28	B	608	CLA	CBD-CGD-O2D-CED
28	B	610	CLA	CBD-CGD-O2D-CED
28	B	611	CLA	CBD-CGD-O2D-CED
28	B	613	CLA	CBD-CGD-O2D-CED
28	B	614	CLA	CBD-CGD-O2D-CED
28	B	616	CLA	CBD-CGD-O2D-CED
28	C	501	CLA	CBD-CGD-O2D-CED
28	C	507	CLA	CBD-CGD-O2D-CED
28	C	509	CLA	CBD-CGD-O2D-CED
28	C	510	CLA	CBD-CGD-O2D-CED
28	C	512	CLA	CBD-CGD-O2D-CED
28	N	602	CLA	CBD-CGD-O2D-CED
28	N	610	CLA	CBD-CGD-O2D-CED
28	N	613	CLA	CBD-CGD-O2D-CED
28	N	614	CLA	CBD-CGD-O2D-CED
28	G	602	CLA	CBD-CGD-O2D-CED
28	G	604	CLA	CBD-CGD-O2D-CED
28	G	612	CLA	CBD-CGD-O2D-CED
28	G	613	CLA	CBD-CGD-O2D-CED
28	S	603	CLA	CBD-CGD-O2D-CED
28	S	605	CLA	CBD-CGD-O2D-CED
28	S	613	CLA	CBD-CGD-O2D-CED
28	S	617	CLA	CBD-CGD-O2D-CED
28	Y	603	CLA	CBD-CGD-O2D-CED
28	Y	608	CLA	CBD-CGD-O2D-CED
28	Y	611	CLA	CBD-CGD-O2D-CED
28	Y	612	CLA	CBD-CGD-O2D-CED
28	Y	613	CLA	CBD-CGD-O2D-CED
28	b	602	CLA	CBD-CGD-O2D-CED
28	b	605	CLA	CBD-CGD-O2D-CED
28	b	608	CLA	CBD-CGD-O2D-CED
28	b	609	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	b	610	CLA	CBD-CGD-O2D-CED
28	b	612	CLA	CBD-CGD-O2D-CED
28	b	613	CLA	CBD-CGD-O2D-CED
28	b	614	CLA	CBD-CGD-O2D-CED
28	b	615	CLA	CBD-CGD-O2D-CED
28	b	616	CLA	CBD-CGD-O2D-CED
28	b	617	CLA	CBD-CGD-O2D-CED
28	c	504	CLA	CBD-CGD-O2D-CED
28	c	507	CLA	CBD-CGD-O2D-CED
28	c	511	CLA	CBD-CGD-O2D-CED
28	c	513	CLA	CBD-CGD-O2D-CED
28	d	403	CLA	CBD-CGD-O2D-CED
29	a	409	PHO	CBD-CGD-O2D-CED
28	C	512	CLA	O1A-CGA-O2A-C1
28	N	603	CLA	O1A-CGA-O2A-C1
28	G	611	CLA	O1A-CGA-O2A-C1
28	S	605	CLA	O1A-CGA-O2A-C1
28	S	613	CLA	O1A-CGA-O2A-C1
28	b	603	CLA	O1A-CGA-O2A-C1
31	c	526	SQD	O10-C23-O48-C46
45	I	102	4RF	O17-C16-O18-C19
28	A	405	CLA	O1D-CGD-O2D-CED
28	B	608	CLA	O1D-CGD-O2D-CED
28	B	614	CLA	O1D-CGD-O2D-CED
28	C	504	CLA	O1D-CGD-O2D-CED
28	N	612	CLA	O1D-CGD-O2D-CED
28	S	604	CLA	O1D-CGD-O2D-CED
28	S	609	CLA	O1D-CGD-O2D-CED
28	S	617	CLA	O1D-CGD-O2D-CED
28	Y	610	CLA	O1D-CGD-O2D-CED
28	b	602	CLA	O1D-CGD-O2D-CED
28	b	610	CLA	O1D-CGD-O2D-CED
28	b	612	CLA	O1D-CGD-O2D-CED
28	b	615	CLA	O1D-CGD-O2D-CED
28	c	501	CLA	O1D-CGD-O2D-CED
28	c	504	CLA	O1D-CGD-O2D-CED
28	c	513	CLA	O1D-CGD-O2D-CED
28	d	402	CLA	O1D-CGD-O2D-CED
35	c	518	DGD	C2G-C1G-O1G-C1A
28	B	604	CLA	O1D-CGD-O2D-CED
28	B	606	CLA	O1D-CGD-O2D-CED
28	B	607	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	B	612	CLA	O1D-CGD-O2D-CED
28	B	615	CLA	O1D-CGD-O2D-CED
28	C	503	CLA	O1D-CGD-O2D-CED
28	C	506	CLA	O1D-CGD-O2D-CED
28	C	511	CLA	O1D-CGD-O2D-CED
28	C	513	CLA	O1D-CGD-O2D-CED
28	N	614	CLA	O1D-CGD-O2D-CED
28	G	603	CLA	O1D-CGD-O2D-CED
28	G	610	CLA	O1D-CGD-O2D-CED
28	S	610	CLA	O1D-CGD-O2D-CED
28	Y	604	CLA	O1D-CGD-O2D-CED
28	b	603	CLA	O1D-CGD-O2D-CED
28	b	604	CLA	O1D-CGD-O2D-CED
28	b	606	CLA	O1D-CGD-O2D-CED
28	c	502	CLA	O1D-CGD-O2D-CED
28	c	506	CLA	O1D-CGD-O2D-CED
28	c	511	CLA	O1D-CGD-O2D-CED
28	N	611	CLA	CBA-CGA-O2A-C1
28	G	604	CLA	CBA-CGA-O2A-C1
28	S	605	CLA	CBA-CGA-O2A-C1
32	W	201	LMG	C29-C28-O8-C9
36	t	101	3PH	C32-C31-O31-C3
45	I	102	4RF	C15-C16-O18-C19
51	Y	627	PTY	O30-C30-O4-C1
28	B	609	CLA	CBD-CGD-O2D-CED
28	B	617	CLA	CBD-CGD-O2D-CED
28	D	402	CLA	CBD-CGD-O2D-CED
28	N	603	CLA	CBD-CGD-O2D-CED
28	N	604	CLA	CBD-CGD-O2D-CED
28	N	611	CLA	CBD-CGD-O2D-CED
28	G	611	CLA	CBD-CGD-O2D-CED
28	S	602	CLA	CBD-CGD-O2D-CED
28	Y	602	CLA	CBD-CGD-O2D-CED
28	a	407	CLA	CBD-CGD-O2D-CED
28	a	410	CLA	CBD-CGD-O2D-CED
28	c	503	CLA	CBD-CGD-O2D-CED
28	A	406	CLA	O1A-CGA-O2A-C1
28	B	603	CLA	O1A-CGA-O2A-C1
28	C	505	CLA	O1A-CGA-O2A-C1
28	N	611	CLA	O1A-CGA-O2A-C1
28	G	604	CLA	O1A-CGA-O2A-C1
28	G	614	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	S	609	CLA	O1A-CGA-O2A-C1
28	S	617	CLA	O1A-CGA-O2A-C1
28	Y	602	CLA	O1A-CGA-O2A-C1
28	Y	604	CLA	O1A-CGA-O2A-C1
28	Y	608	CLA	O1A-CGA-O2A-C1
28	Y	611	CLA	O1A-CGA-O2A-C1
28	c	505	CLA	O1A-CGA-O2A-C1
28	c	506	CLA	O1A-CGA-O2A-C1
32	C	521	LMG	O10-C28-O8-C9
32	c	521	LMG	O10-C28-O8-C9
32	c	523	LMG	O10-C28-O8-C9
36	T	101	3PH	O32-C31-O31-C3
36	b	624	3PH	O32-C31-O31-C3
36	t	101	3PH	O32-C31-O31-C3
45	i	101	4RF	O17-C16-O18-C19
28	D	403	CLA	O1D-CGD-O2D-CED
28	S	611	CLA	O1D-CGD-O2D-CED
28	Y	614	CLA	O1D-CGD-O2D-CED
28	b	607	CLA	O1D-CGD-O2D-CED
28	b	611	CLA	O1D-CGD-O2D-CED
32	d	411	LMG	C4-C5-C6-O5
28	B	603	CLA	O1D-CGD-O2D-CED
28	C	502	CLA	O1D-CGD-O2D-CED
28	S	612	CLA	O1D-CGD-O2D-CED
28	S	614	CLA	O1D-CGD-O2D-CED
28	c	509	CLA	O1D-CGD-O2D-CED
28	c	510	CLA	O1D-CGD-O2D-CED
51	Y	627	PTY	C31-C30-O4-C1
28	c	512	CLA	CBD-CGD-O2D-CED
28	N	610	CLA	O1D-CGD-O2D-CED
28	G	614	CLA	O1D-CGD-O2D-CED
28	Y	603	CLA	O1D-CGD-O2D-CED
32	W	201	LMG	O9-C10-O7-C8
32	a	413	LMG	O9-C10-O7-C8
32	c	523	LMG	O9-C10-O7-C8
36	T	101	3PH	O22-C21-O21-C2
38	S	624	LHG	O9-C7-O7-C5
45	i	101	4RF	O23-C22-O21-C20
51	Y	627	PTY	O10-C8-O7-C6
28	d	403	CLA	O1D-CGD-O2D-CED
28	B	605	CLA	C3-C5-C6-C7
28	B	608	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	B	610	CLA	C3-C5-C6-C7
28	S	613	CLA	C3-C5-C6-C7
28	b	617	CLA	C3-C5-C6-C7
28	c	504	CLA	C3-C5-C6-C7
28	c	508	CLA	C3-C5-C6-C7
28	d	403	CLA	C3-C5-C6-C7
29	A	409	PHO	C3-C5-C6-C7
28	A	406	CLA	CBA-CGA-O2A-C1
28	B	603	CLA	CBA-CGA-O2A-C1
28	B	608	CLA	CBA-CGA-O2A-C1
28	C	505	CLA	CBA-CGA-O2A-C1
28	C	509	CLA	CBA-CGA-O2A-C1
28	D	403	CLA	CBA-CGA-O2A-C1
28	N	603	CLA	CBA-CGA-O2A-C1
28	G	611	CLA	CBA-CGA-O2A-C1
28	S	610	CLA	CBA-CGA-O2A-C1
28	S	613	CLA	CBA-CGA-O2A-C1
28	S	617	CLA	CBA-CGA-O2A-C1
28	Y	603	CLA	CBA-CGA-O2A-C1
28	Y	604	CLA	CBA-CGA-O2A-C1
28	Y	611	CLA	CBA-CGA-O2A-C1
28	b	603	CLA	CBA-CGA-O2A-C1
28	c	505	CLA	CBA-CGA-O2A-C1
28	c	511	CLA	CBA-CGA-O2A-C1
31	c	526	SQD	C24-C23-O48-C46
32	C	521	LMG	C29-C28-O8-C9
32	c	521	LMG	C29-C28-O8-C9
36	T	101	3PH	C32-C31-O31-C3
45	i	101	4RF	C15-C16-O18-C19
32	a	413	LMG	C11-C10-O7-C8
35	B	623	DGD	C2B-C1B-O2G-C2G
35	b	623	DGD	C2B-C1B-O2G-C2G
36	T	101	3PH	C22-C21-O21-C2
28	N	602	CLA	O1D-CGD-O2D-CED
28	a	406	CLA	CBD-CGD-O2D-CED
31	b	626	SQD	O10-C23-O48-C46
28	B	606	CLA	C4-C3-C5-C6
28	c	504	CLA	C4-C3-C5-C6
46	N	606	CHL	C4-C3-C5-C6
28	G	613	CLA	C2A-CAA-CBA-CGA
28	G	614	CLA	C2A-CAA-CBA-CGA
28	S	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
28	S	614	CLA	C2A-CAA-CBA-CGA
28	c	507	CLA	C2A-CAA-CBA-CGA
28	C	506	CLA	O1A-CGA-O2A-C1
32	A	413	LMG	C17-C18-C19-C20
32	A	413	LMG	C35-C36-C37-C38
32	A	413	LMG	C38-C39-C40-C41
32	B	622	LMG	C17-C18-C19-C20
32	C	521	LMG	C17-C18-C19-C20
32	C	521	LMG	C35-C36-C37-C38
32	C	523	LMG	C17-C18-C19-C20
32	C	523	LMG	C41-C42-C43-C44
32	D	411	LMG	C17-C18-C19-C20
32	D	411	LMG	C20-C21-C22-C23
32	H	102	LMG	C38-C39-C40-C41
32	W	201	LMG	C35-C36-C37-C38
32	W	201	LMG	C38-C39-C40-C41
32	a	413	LMG	C17-C18-C19-C20
32	a	413	LMG	C35-C36-C37-C38
32	a	413	LMG	C38-C39-C40-C41
32	b	622	LMG	C17-C18-C19-C20
32	c	521	LMG	C17-C18-C19-C20
32	c	521	LMG	C35-C36-C37-C38
32	c	523	LMG	C17-C18-C19-C20
32	c	523	LMG	C41-C42-C43-C44
32	d	411	LMG	C17-C18-C19-C20
32	d	411	LMG	C20-C21-C22-C23
32	h	102	LMG	C38-C39-C40-C41
32	w	201	LMG	C35-C36-C37-C38
32	w	201	LMG	C38-C39-C40-C41
35	C	518	DGD	C8B-C9B-CAB-CBB
35	C	519	DGD	C8A-C9A-CAA-CBA
35	C	519	DGD	CBB-CCB-CDB-CEB
35	C	520	DGD	CBB-CCB-CDB-CEB
35	c	518	DGD	C8B-C9B-CAB-CBB
35	c	519	DGD	C8A-C9A-CAA-CBA
35	c	519	DGD	CBB-CCB-CDB-CEB
35	c	520	DGD	CBB-CCB-CDB-CEB
28	N	610	CLA	C3-C5-C6-C7
28	G	611	CLA	C3-C5-C6-C7
28	G	613	CLA	C3-C5-C6-C7
28	S	610	CLA	C3-C5-C6-C7
28	Y	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	b	604	CLA	C3-C5-C6-C7
28	b	605	CLA	C3-C5-C6-C7
28	N	602	CLA	CBA-CGA-O2A-C1
28	G	614	CLA	CBA-CGA-O2A-C1
28	S	609	CLA	CBA-CGA-O2A-C1
28	Y	602	CLA	CBA-CGA-O2A-C1
28	Y	608	CLA	CBA-CGA-O2A-C1
28	a	407	CLA	CBA-CGA-O2A-C1
28	b	606	CLA	CBA-CGA-O2A-C1
28	b	608	CLA	CBA-CGA-O2A-C1
28	b	611	CLA	CBA-CGA-O2A-C1
28	c	506	CLA	CBA-CGA-O2A-C1
32	c	523	LMG	C29-C28-O8-C9
35	B	623	DGD	C2A-C1A-O1G-C1G
36	b	624	3PH	C32-C31-O31-C3
32	d	411	LMG	O6-C5-C6-O5
28	C	510	CLA	O1D-CGD-O2D-CED
28	G	602	CLA	O1D-CGD-O2D-CED
28	S	605	CLA	O1D-CGD-O2D-CED
28	Y	611	CLA	O1D-CGD-O2D-CED
28	B	610	CLA	O1D-CGD-O2D-CED
28	B	613	CLA	O1D-CGD-O2D-CED
28	B	616	CLA	O1D-CGD-O2D-CED
28	C	509	CLA	O1D-CGD-O2D-CED
28	Y	612	CLA	O1D-CGD-O2D-CED
28	b	609	CLA	O1D-CGD-O2D-CED
36	b	624	3PH	O22-C21-O21-C2
45	I	102	4RF	O23-C22-O21-C20
41	d	405	PL9	C22-C23-C24-C26
41	d	405	PL9	C37-C38-C39-C41
28	G	602	CLA	O1A-CGA-O2A-C1
28	G	613	CLA	O1A-CGA-O2A-C1
28	S	602	CLA	O1A-CGA-O2A-C1
28	Y	603	CLA	O1A-CGA-O2A-C1
28	a	406	CLA	O1A-CGA-O2A-C1
28	b	611	CLA	O1A-CGA-O2A-C1
28	c	509	CLA	O1A-CGA-O2A-C1
32	C	523	LMG	O10-C28-O8-C9
28	A	410	CLA	O1D-CGD-O2D-CED
28	B	611	CLA	O1D-CGD-O2D-CED
28	C	512	CLA	O1D-CGD-O2D-CED
28	c	507	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	B	618	BCR	C9-C10-C11-C12
30	b	619	BCR	C9-C10-C11-C12
43	h	101	RRX	C15-C16-C17-C18
28	C	507	CLA	O1D-CGD-O2D-CED
38	D	409	LHG	O2-C2-C3-O3
38	G	624	LHG	O2-C2-C3-O3
38	Y	624	LHG	O2-C2-C3-O3
38	c	525	LHG	O2-C2-C3-O3
38	l	101	LHG	O2-C2-C3-O3
50	S	625	LPX	O1-C3-C4-O5
28	C	506	CLA	C3-C5-C6-C7
28	b	608	CLA	C3-C5-C6-C7
28	A	407	CLA	CBA-CGA-O2A-C1
28	B	613	CLA	CBA-CGA-O2A-C1
28	G	602	CLA	CBA-CGA-O2A-C1
28	G	613	CLA	CBA-CGA-O2A-C1
28	S	602	CLA	CBA-CGA-O2A-C1
28	Y	612	CLA	CBA-CGA-O2A-C1
28	Y	613	CLA	CBA-CGA-O2A-C1
28	a	410	CLA	CBA-CGA-O2A-C1
28	c	501	CLA	CBA-CGA-O2A-C1
28	c	509	CLA	CBA-CGA-O2A-C1
31	b	626	SQD	C24-C23-O48-C46
38	l	101	LHG	C24-C23-O8-C6
28	B	608	CLA	O1A-CGA-O2A-C1
28	C	509	CLA	O1A-CGA-O2A-C1
28	S	610	CLA	O1A-CGA-O2A-C1
28	Y	612	CLA	O1A-CGA-O2A-C1
28	c	511	CLA	O1A-CGA-O2A-C1
38	l	101	LHG	O10-C23-O8-C6
28	S	603	CLA	O1D-CGD-O2D-CED
28	b	616	CLA	O1D-CGD-O2D-CED
28	b	617	CLA	O1D-CGD-O2D-CED
50	S	625	LPX	O5-C4-C5-O6
31	m	101	SQD	C8-C7-O47-C45
32	C	523	LMG	C11-C10-O7-C8
36	b	624	3PH	C22-C21-O21-C2
38	N	624	LHG	C8-C7-O7-C5
28	G	604	CLA	O1D-CGD-O2D-CED
28	b	605	CLA	O1D-CGD-O2D-CED
38	C	525	LHG	C11-C12-C13-C14
28	Y	613	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
38	c	525	LHG	C11-C12-C13-C14
28	C	501	CLA	O1D-CGD-O2D-CED
28	G	612	CLA	O1D-CGD-O2D-CED
28	S	609	CLA	C3-C5-C6-C7
28	c	509	CLA	C3-C5-C6-C7
28	c	511	CLA	C3-C5-C6-C7
28	c	512	CLA	C3-C5-C6-C7
28	d	402	CLA	C3-C5-C6-C7
28	C	506	CLA	CBA-CGA-O2A-C1
28	N	610	CLA	CBA-CGA-O2A-C1
28	a	406	CLA	CBA-CGA-O2A-C1
32	C	523	LMG	C29-C28-O8-C9
28	A	407	CLA	O1A-CGA-O2A-C1
28	B	613	CLA	O1A-CGA-O2A-C1
28	c	501	CLA	O1A-CGA-O2A-C1
42	f	101	HEM	C3D-CAD-CBD-CGD
28	C	507	CLA	C4-C3-C5-C6
28	c	501	CLA	C4-C3-C5-C6
28	d	402	CLA	C4-C3-C5-C6
28	C	507	CLA	C2-C3-C5-C6
28	b	606	CLA	C2-C3-C5-C6
28	c	501	CLA	C2-C3-C5-C6
28	d	402	CLA	C2-C3-C5-C6
28	N	602	CLA	C2A-CAA-CBA-CGA
28	c	502	CLA	C2A-CAA-CBA-CGA
28	b	613	CLA	O1D-CGD-O2D-CED
29	a	409	PHO	O1D-CGD-O2D-CED
28	B	610	CLA	O1A-CGA-O2A-C1
28	N	602	CLA	O1A-CGA-O2A-C1
28	a	407	CLA	O1A-CGA-O2A-C1
28	b	606	CLA	O1A-CGA-O2A-C1
28	b	608	CLA	O1A-CGA-O2A-C1
35	B	623	DGD	O1A-C1A-O1G-C1G
31	a	412	SQD	O5-C1-O6-C44
32	b	622	LMG	O6-C1-O1-C7
41	d	405	PL9	C9-C11-C12-C13
41	d	405	PL9	C19-C21-C22-C23
41	d	405	PL9	C39-C41-C42-C43
28	B	606	CLA	CBA-CGA-O2A-C1
28	B	610	CLA	CBA-CGA-O2A-C1
28	C	511	CLA	CBA-CGA-O2A-C1
36	S	626	3PH	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
45	K	101	4RF	C43-C41-O40-C39
38	l	101	LHG	C7-C8-C9-C10
45	I	102	4RF	C33-C34-C35-C36
28	B	617	CLA	O1D-CGD-O2D-CED
28	Y	602	CLA	O1D-CGD-O2D-CED
28	a	407	CLA	O1D-CGD-O2D-CED
28	a	410	CLA	O1D-CGD-O2D-CED
28	a	410	CLA	O1A-CGA-O2A-C1
31	B	621	SQD	C8-C7-O47-C45
28	N	603	CLA	O1D-CGD-O2D-CED
28	N	604	CLA	O1D-CGD-O2D-CED
28	B	602	CLA	CBD-CGD-O2D-CED
38	L	101	LHG	C1-C2-C3-O3
38	G	624	LHG	C1-C2-C3-O3
38	S	624	LHG	C1-C2-C3-O3
38	l	101	LHG	C1-C2-C3-O3
31	B	621	SQD	O49-C7-O47-C45
31	m	101	SQD	O49-C7-O47-C45
38	N	624	LHG	O9-C7-O7-C5
28	C	511	CLA	O1A-CGA-O2A-C1
28	D	403	CLA	C3-C5-C6-C7
28	S	603	CLA	C3-C5-C6-C7
28	c	506	CLA	C3-C5-C6-C7
28	N	611	CLA	O1D-CGD-O2D-CED
28	A	405	CLA	CBA-CGA-O2A-C1
28	B	604	CLA	CBA-CGA-O2A-C1
28	B	611	CLA	CBA-CGA-O2A-C1
28	C	503	CLA	CBA-CGA-O2A-C1
28	b	610	CLA	CBA-CGA-O2A-C1
28	b	613	CLA	CBA-CGA-O2A-C1
28	b	614	CLA	CBA-CGA-O2A-C1
28	c	503	CLA	CBA-CGA-O2A-C1
28	c	508	CLA	CBA-CGA-O2A-C1
28	c	510	CLA	CBA-CGA-O2A-C1
28	d	402	CLA	CBA-CGA-O2A-C1
31	C	526	SQD	C24-C23-O48-C46
31	M	101	SQD	C24-C23-O48-C46
31	m	101	SQD	C24-C23-O48-C46
35	C	520	DGD	C2A-C1A-O1G-C1G
35	c	518	DGD	C2A-C1A-O1G-C1G
36	B	624	3PH	C32-C31-O31-C3
38	L	101	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
43	H	101	RRX	C9-C10-C11-C12
28	G	610	CLA	C13-C15-C16-C17
28	S	611	CLA	C5-C6-C7-C8
28	N	610	CLA	O1A-CGA-O2A-C1
41	d	405	PL9	C47-C48-C49-C51
45	I	102	4RF	C31-C32-C33-C34
28	S	602	CLA	O1D-CGD-O2D-CED
36	t	101	3PH	O11-C1-C2-O21
31	b	621	SQD	C10-C11-C12-C13
28	B	602	CLA	C15-C16-C17-C18
28	B	604	CLA	C10-C11-C12-C13
28	B	607	CLA	C10-C11-C12-C13
28	B	608	CLA	C8-C10-C11-C12
28	B	610	CLA	C5-C6-C7-C8
28	B	611	CLA	C15-C16-C17-C18
28	N	613	CLA	C15-C16-C17-C18
28	G	603	CLA	C5-C6-C7-C8
28	S	603	CLA	C5-C6-C7-C8
28	S	613	CLA	C5-C6-C7-C8
28	b	604	CLA	C15-C16-C17-C18
28	b	611	CLA	C15-C16-C17-C18
28	b	613	CLA	C10-C11-C12-C13
28	c	503	CLA	C13-C15-C16-C17
38	D	410	LHG	C7-C8-C9-C10
45	I	102	4RF	C13-C14-C15-C16
31	a	412	SQD	C2-C1-O6-C44
31	c	526	SQD	C2-C1-O6-C44
35	B	623	DGD	C2D-C1D-O3G-C3G
35	b	623	DGD	C2D-C1D-O3G-C3G
28	B	611	CLA	O1A-CGA-O2A-C1
28	C	503	CLA	O1A-CGA-O2A-C1
31	C	526	SQD	O10-C23-O48-C46
31	M	101	SQD	O10-C23-O48-C46
31	m	101	SQD	O10-C23-O48-C46
28	C	501	CLA	C4-C3-C5-C6
28	B	606	CLA	C2-C3-C5-C6
28	A	405	CLA	C11-C12-C13-C14
28	B	603	CLA	C14-C13-C15-C16
28	B	605	CLA	C6-C7-C8-C9
28	C	505	CLA	C11-C10-C8-C9
28	C	513	CLA	C11-C10-C8-C9
28	D	402	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	b	602	CLA	C11-C12-C13-C14
28	b	604	CLA	C14-C13-C15-C16
28	b	605	CLA	C6-C7-C8-C9
28	b	606	CLA	C6-C7-C8-C9
28	b	608	CLA	C11-C10-C8-C9
28	b	612	CLA	C11-C12-C13-C14
28	b	616	CLA	C11-C10-C8-C9
28	d	402	CLA	C6-C7-C8-C9
28	d	403	CLA	C14-C13-C15-C16
46	N	606	CHL	C14-C13-C15-C16
46	G	609	CHL	C11-C10-C8-C9
46	Y	609	CHL	C11-C12-C13-C14
28	D	402	CLA	O1D-CGD-O2D-CED
28	B	615	CLA	C10-C11-C12-C13
28	D	403	CLA	C5-C6-C7-C8
28	Y	602	CLA	C2A-CAA-CBA-CGA
28	a	407	CLA	C2A-CAA-CBA-CGA
30	B	619	BCR	C36-C18-C19-C20
30	C	516	BCR	C36-C18-C19-C20
30	C	517	BCR	C37-C22-C23-C24
30	b	618	BCR	C36-C18-C19-C20
30	c	515	BCR	C11-C12-C13-C35
30	c	515	BCR	C36-C18-C19-C20
34	b	620	C7Z	C7-C8-C9-C19
43	H	101	RRX	C7-C8-C9-C34
47	Y	620	LUT	C31-C32-C33-C40
49	Y	623	NEX	C11-C12-C13-C20
30	C	517	BCR	C21-C22-C23-C24
30	c	515	BCR	C7-C8-C9-C10
34	b	620	C7Z	C7-C8-C9-C10
43	H	101	RRX	C7-C8-C9-C10
32	C	523	LMG	O9-C10-O7-C8
45	K	101	4RF	C31-C32-C33-C34
31	a	412	SQD	C7-C8-C9-C10
38	d	409	LHG	C7-C8-C9-C10
28	A	405	CLA	O1A-CGA-O2A-C1
28	B	604	CLA	O1A-CGA-O2A-C1
28	B	613	CLA	C10-C11-C12-C13
28	S	609	CLA	C10-C11-C12-C13
28	Y	612	CLA	C8-C10-C11-C12
28	b	602	CLA	C15-C16-C17-C18
28	b	609	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	c	505	CLA	C10-C11-C12-C13
28	c	506	CLA	C13-C15-C16-C17
28	c	508	CLA	C15-C16-C17-C18
45	k	101	4RF	C12-C13-C14-C15
28	S	604	CLA	C3-C5-C6-C7
28	B	614	CLA	CBA-CGA-O2A-C1
28	b	604	CLA	CBA-CGA-O2A-C1
37	C	524	DGA	CA2-CA1-OG1-CG1
45	i	101	4RF	C43-C41-O40-C39
28	B	604	CLA	C13-C15-C16-C17
28	B	608	CLA	C13-C15-C16-C17
28	C	502	CLA	C13-C15-C16-C17
28	C	504	CLA	C10-C11-C12-C13
28	C	512	CLA	C13-C15-C16-C17
28	C	513	CLA	C10-C11-C12-C13
28	N	602	CLA	C8-C10-C11-C12
28	G	613	CLA	C13-C15-C16-C17
28	S	611	CLA	C8-C10-C11-C12
28	Y	603	CLA	C13-C15-C16-C17
28	Y	604	CLA	C8-C10-C11-C12
28	Y	610	CLA	C13-C15-C16-C17
28	Y	613	CLA	C5-C6-C7-C8
28	Y	613	CLA	C15-C16-C17-C18
28	Y	614	CLA	C8-C10-C11-C12
28	b	603	CLA	C5-C6-C7-C8
28	b	605	CLA	C8-C10-C11-C12
28	b	606	CLA	C15-C16-C17-C18
28	d	403	CLA	C8-C10-C11-C12
37	j	101	DGA	CB1-CB2-CB3-CB4
38	G	624	LHG	C7-C8-C9-C10
38	d	409	LHG	C23-C24-C25-C26
38	l	101	LHG	C23-C24-C25-C26
51	Y	626	PTY	C8-C11-C12-C13
28	B	605	CLA	C15-C16-C17-C18
28	B	614	CLA	C5-C6-C7-C8
28	C	510	CLA	C15-C16-C17-C18
28	C	512	CLA	C5-C6-C7-C8
28	N	602	CLA	C15-C16-C17-C18
28	N	613	CLA	C13-C15-C16-C17
28	G	603	CLA	C15-C16-C17-C18
28	S	603	CLA	C13-C15-C16-C17
28	Y	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	Y	602	CLA	C13-C15-C16-C17
28	b	602	CLA	C10-C11-C12-C13
28	b	612	CLA	C5-C6-C7-C8
28	b	617	CLA	C13-C15-C16-C17
28	c	501	CLA	C13-C15-C16-C17
28	c	503	CLA	C15-C16-C17-C18
28	c	510	CLA	C15-C16-C17-C18
28	c	511	CLA	C8-C10-C11-C12
28	c	512	CLA	C5-C6-C7-C8
28	B	609	CLA	O1D-CGD-O2D-CED
28	c	503	CLA	O1D-CGD-O2D-CED
38	D	410	LHG	O1-C1-C2-O2
38	l	101	LHG	O1-C1-C2-O2
36	B	624	3PH	O32-C31-O31-C3
31	B	621	SQD	C23-C24-C25-C26
32	A	413	LMG	C10-C11-C12-C13
32	H	102	LMG	C28-C29-C30-C31
32	b	622	LMG	C10-C11-C12-C13
32	b	622	LMG	C28-C29-C30-C31
32	h	102	LMG	C28-C29-C30-C31
35	C	518	DGD	C1B-C2B-C3B-C4B
36	S	626	3PH	C31-C32-C33-C34
37	C	524	DGA	CB1-CB2-CB3-CB4
37	J	101	DGA	CB1-CB2-CB3-CB4
37	c	524	DGA	CB1-CB2-CB3-CB4
38	C	525	LHG	C23-C24-C25-C26
38	D	408	LHG	C7-C8-C9-C10
38	D	409	LHG	C7-C8-C9-C10
38	D	410	LHG	C23-C24-C25-C26
38	N	624	LHG	C7-C8-C9-C10
38	c	525	LHG	C23-C24-C25-C26
38	d	408	LHG	C23-C24-C25-C26
38	d	410	LHG	C7-C8-C9-C10
38	d	410	LHG	C23-C24-C25-C26
45	I	102	4RF	C22-C24-C25-C26
45	i	101	4RF	C13-C14-C15-C16
45	k	101	4RF	C22-C24-C25-C26
28	B	614	CLA	C13-C15-C16-C17
28	C	508	CLA	C15-C16-C17-C18
28	N	613	CLA	C5-C6-C7-C8
28	G	602	CLA	C8-C10-C11-C12
28	G	610	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	Y	610	CLA	C8-C10-C11-C12
28	Y	611	CLA	C10-C11-C12-C13
28	b	606	CLA	C8-C10-C11-C12
28	c	508	CLA	C5-C6-C7-C8
28	c	512	CLA	C15-C16-C17-C18
28	B	603	CLA	C3-C5-C6-C7
28	Y	614	CLA	CBA-CGA-O2A-C1
28	c	504	CLA	CBA-CGA-O2A-C1
28	G	611	CLA	O1D-CGD-O2D-CED
28	A	406	CLA	C2-C1-O2A-CGA
28	B	602	CLA	C2-C1-O2A-CGA
28	B	608	CLA	C2-C1-O2A-CGA
28	B	614	CLA	C2-C1-O2A-CGA
28	C	509	CLA	C2-C1-O2A-CGA
28	N	611	CLA	C2-C1-O2A-CGA
28	G	604	CLA	C2-C1-O2A-CGA
28	G	611	CLA	C2-C1-O2A-CGA
28	G	614	CLA	C2-C1-O2A-CGA
28	Y	603	CLA	C2-C1-O2A-CGA
28	Y	604	CLA	C2-C1-O2A-CGA
28	Y	614	CLA	C2-C1-O2A-CGA
28	a	407	CLA	C2-C1-O2A-CGA
28	b	602	CLA	C2-C1-O2A-CGA
28	b	605	CLA	C2-C1-O2A-CGA
28	b	608	CLA	C2-C1-O2A-CGA
28	b	614	CLA	C2-C1-O2A-CGA
28	B	608	CLA	C5-C6-C7-C8
28	B	609	CLA	C5-C6-C7-C8
28	N	603	CLA	C13-C15-C16-C17
28	N	604	CLA	C10-C11-C12-C13
28	N	613	CLA	C8-C10-C11-C12
28	G	603	CLA	C8-C10-C11-C12
28	Y	604	CLA	C13-C15-C16-C17
28	b	615	CLA	C10-C11-C12-C13
28	b	617	CLA	C10-C11-C12-C13
31	c	526	SQD	C7-C8-C9-C10
45	k	101	4RF	C41-C43-C44-C45
28	A	406	CLA	CBD-CGD-O2D-CED
46	G	608	CHL	C2A-CAA-CBA-CGA
31	c	526	SQD	C8-C7-O47-C45
28	C	503	CLA	C15-C16-C17-C18
28	C	506	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	G	611	CLA	C10-C11-C12-C13
28	A	406	CLA	C11-C12-C13-C15
28	b	604	CLA	C11-C12-C13-C15
46	G	601	CHL	C12-C13-C15-C16
28	a	406	CLA	C3-C5-C6-C7
28	B	606	CLA	O1A-CGA-O2A-C1
28	b	610	CLA	O1A-CGA-O2A-C1
28	b	614	CLA	O1A-CGA-O2A-C1
28	c	508	CLA	O1A-CGA-O2A-C1
28	c	510	CLA	O1A-CGA-O2A-C1
28	d	402	CLA	O1A-CGA-O2A-C1
38	L	101	LHG	O10-C23-O8-C6
30	B	619	BCR	C19-C20-C21-C22
30	b	618	BCR	C9-C10-C11-C12
30	c	514	BCR	C15-C16-C17-C18
30	c	516	BCR	C19-C20-C21-C22
30	c	517	BCR	C9-C10-C11-C12
30	d	404	BCR	C9-C10-C11-C12
47	G	621	LUT	C29-C30-C31-C32
47	S	621	LUT	C29-C30-C31-C32
28	A	407	CLA	C2A-CAA-CBA-CGA
28	B	602	CLA	C2A-CAA-CBA-CGA
29	A	408	PHO	C2A-CAA-CBA-CGA
46	N	606	CHL	C2A-CAA-CBA-CGA
46	S	608	CHL	C2A-CAA-CBA-CGA
46	Y	607	CHL	C2A-CAA-CBA-CGA
28	c	512	CLA	O1D-CGD-O2D-CED
28	C	510	CLA	C5-C6-C7-C8
28	C	510	CLA	C8-C10-C11-C12
28	C	513	CLA	C8-C10-C11-C12
28	N	602	CLA	C13-C15-C16-C17
28	S	602	CLA	C10-C11-C12-C13
28	b	604	CLA	C8-C10-C11-C12
28	b	607	CLA	C10-C11-C12-C13
28	b	612	CLA	C8-C10-C11-C12
28	b	615	CLA	C15-C16-C17-C18
28	c	504	CLA	C13-C15-C16-C17
28	c	504	CLA	C15-C16-C17-C18
38	c	525	LHG	C33-C34-C35-C36
28	b	613	CLA	O1A-CGA-O2A-C1
28	c	503	CLA	O1A-CGA-O2A-C1
35	C	520	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
35	c	518	DGD	O1A-C1A-O1G-C1G
31	B	626	SQD	O5-C1-O6-C44
35	C	519	DGD	O6E-C1E-O5D-C6D
28	G	602	CLA	C13-C15-C16-C17
28	c	506	CLA	C8-C10-C11-C12
38	S	624	LHG	C9-C10-C11-C12
35	c	518	DGD	C1B-C2B-C3B-C4B
30	c	515	BCR	C10-C11-C12-C13
48	Y	622	XAT	C10-C11-C12-C13
49	Y	623	NEX	C30-C31-C32-C33
38	C	525	LHG	O2-C2-C3-O3
38	L	101	LHG	O2-C2-C3-O3
38	d	408	LHG	O2-C2-C3-O3
31	M	101	SQD	O49-C7-O47-C45
31	b	621	SQD	O49-C7-O47-C45
28	B	608	CLA	C15-C16-C17-C18
28	B	610	CLA	C8-C10-C11-C12
28	B	617	CLA	C15-C16-C17-C18
28	C	508	CLA	C13-C15-C16-C17
28	N	603	CLA	C8-C10-C11-C12
28	G	611	CLA	C15-C16-C17-C18
28	Y	611	CLA	C15-C16-C17-C18
28	Y	614	CLA	C5-C6-C7-C8
28	b	608	CLA	C10-C11-C12-C13
28	c	501	CLA	C15-C16-C17-C18
28	c	512	CLA	C10-C11-C12-C13
36	S	626	3PH	O32-C31-O31-C3
38	C	525	LHG	C33-C34-C35-C36
38	D	409	LHG	C9-C10-C11-C12
28	A	410	CLA	C8-C10-C11-C12
28	A	410	CLA	C10-C11-C12-C13
28	B	612	CLA	C15-C16-C17-C18
28	C	502	CLA	C5-C6-C7-C8
28	C	508	CLA	C5-C6-C7-C8
28	b	609	CLA	C8-C10-C11-C12
28	b	615	CLA	C5-C6-C7-C8
28	a	406	CLA	O1D-CGD-O2D-CED
28	B	614	CLA	O1A-CGA-O2A-C1
28	c	504	CLA	O1A-CGA-O2A-C1
37	C	524	DGA	OA1-CA1-OG1-CG1
45	K	101	4RF	O42-C41-O40-C39
45	i	101	4RF	O42-C41-O40-C39

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Mol	Chain	Res	Type	Atoms
31	M	101	SQD	C8-C7-O47-C45
31	b	621	SQD	C8-C7-O47-C45
31	b	626	SQD	C8-C7-O47-C45
32	A	413	LMG	C11-C10-O7-C8
38	G	624	LHG	C8-C7-O7-C5
28	B	602	CLA	C13-C15-C16-C17
28	B	612	CLA	C5-C6-C7-C8
28	B	612	CLA	C13-C15-C16-C17
28	C	507	CLA	C15-C16-C17-C18
28	C	508	CLA	C8-C10-C11-C12
28	G	613	CLA	C5-C6-C7-C8
28	S	610	CLA	C10-C11-C12-C13
28	b	610	CLA	C5-C6-C7-C8
28	b	616	CLA	C13-C15-C16-C17
28	c	506	CLA	C5-C6-C7-C8
28	d	403	CLA	C13-C15-C16-C17
46	N	606	CHL	C5-C6-C7-C8
38	C	525	LHG	C4-O6-P-O3
38	D	409	LHG	C4-O6-P-O3
38	D	410	LHG	C3-O3-P-O6
38	D	410	LHG	C4-O6-P-O3
38	N	624	LHG	C4-O6-P-O3
38	G	624	LHG	C4-O6-P-O3
38	Y	624	LHG	C4-O6-P-O3
38	c	525	LHG	C4-O6-P-O3
38	d	408	LHG	C3-O3-P-O6
38	d	410	LHG	C3-O3-P-O6
50	S	625	LPX	C1-O2-P1-O1
51	Y	627	PTY	C5-O14-P1-O11
38	L	101	LHG	C7-C8-C9-C10
28	C	510	CLA	CBA-CGA-O2A-C1
28	a	405	CLA	CBA-CGA-O2A-C1
28	B	608	CLA	C10-C11-C12-C13
28	C	510	CLA	C13-C15-C16-C17
28	d	403	CLA	C10-C11-C12-C13
31	m	101	SQD	C7-C8-C9-C10
38	C	525	LHG	C1-C2-C3-O3
38	D	409	LHG	C1-C2-C3-O3
38	d	408	LHG	C1-C2-C3-O3
31	b	626	SQD	O49-C7-O47-C45
31	c	526	SQD	O49-C7-O47-C45
32	A	413	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
38	G	624	LHG	O9-C7-O7-C5
28	Y	611	CLA	C4-C3-C5-C6
46	N	601	CHL	C4-C3-C5-C6
28	S	609	CLA	C5-C6-C7-C8
28	S	611	CLA	C13-C15-C16-C17
28	Y	602	CLA	C15-C16-C17-C18
28	b	604	CLA	C13-C15-C16-C17
28	c	512	CLA	C13-C15-C16-C17
38	S	624	LHG	C30-C31-C32-C33
28	B	604	CLA	C2A-CAA-CBA-CGA
28	C	505	CLA	C2A-CAA-CBA-CGA
28	C	507	CLA	C2A-CAA-CBA-CGA
28	S	603	CLA	C2A-CAA-CBA-CGA
28	S	613	CLA	C2A-CAA-CBA-CGA
28	Y	613	CLA	C2A-CAA-CBA-CGA
28	c	505	CLA	C2A-CAA-CBA-CGA
28	C	507	CLA	C16-C17-C18-C20
28	D	402	CLA	C16-C17-C18-C19
28	G	613	CLA	C16-C17-C18-C20
28	c	511	CLA	C16-C17-C18-C19
28	B	602	CLA	CBA-CGA-O2A-C1
28	G	603	CLA	CBA-CGA-O2A-C1
38	d	408	LHG	C24-C23-O8-C6
28	D	402	CLA	C15-C16-C17-C18
28	b	608	CLA	C13-C15-C16-C17
47	N	621	LUT	C29-C30-C31-C32
33	a	414	SPH	C5-C6-C7-C8
38	D	409	LHG	C23-C24-C25-C26
37	c	524	DGA	CA4-CA5-CA6-CA7
45	k	101	4RF	C29-C30-C31-C32
32	h	102	LMG	C11-C10-O7-C8
28	C	505	CLA	C8-C10-C11-C12
28	b	604	CLA	C10-C11-C12-C13
49	G	623	NEX	C39-C29-C30-C31
49	G	623	NEX	C40-C33-C34-C35
49	Y	623	NEX	C39-C29-C30-C31
31	A	412	SQD	C13-C14-C15-C16
35	c	519	DGD	C4B-C5B-C6B-C7B
36	B	624	3PH	C29-C2A-C2B-C2C
36	t	101	3PH	C2A-C2B-C2C-C2D
37	C	524	DGA	CB7-CB8-CB9-CAB
37	J	101	DGA	CB7-CB8-CB9-CAB

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Mol	Chain	Res	Type	Atoms
38	D	408	LHG	C30-C31-C32-C33
28	C	509	CLA	C16-C17-C18-C19
28	C	513	CLA	C16-C17-C18-C19
28	b	602	CLA	C16-C17-C18-C20
28	b	609	CLA	C16-C17-C18-C20
28	d	402	CLA	C16-C17-C18-C20
36	B	624	3PH	C3C-C3D-C3E-C3F
36	T	101	3PH	C29-C2A-C2B-C2C
37	B	625	DGA	CB9-CAB-CBB-CCB
37	c	524	DGA	CA2-CA3-CA4-CA5
37	c	524	DGA	CB7-CB8-CB9-CAB
38	C	525	LHG	C29-C30-C31-C32
38	D	408	LHG	C25-C26-C27-C28
38	N	624	LHG	C33-C34-C35-C36
38	S	624	LHG	C12-C13-C14-C15
38	Y	624	LHG	C13-C14-C15-C16
45	I	102	4RF	C46-C47-C48-C49
45	i	101	4RF	C07-C08-C09-C10
45	k	101	4RF	C26-C27-C28-C29
32	h	102	LMG	O9-C10-O7-C8
31	M	101	SQD	C7-C8-C9-C10
31	a	412	SQD	C30-C31-C32-C33
36	b	624	3PH	C37-C38-C39-C3A
37	c	524	DGA	CA5-CA6-CA7-CA8
37	c	524	DGA	CAA-CBA-CCA-CDA
37	c	524	DGA	CEA-CFA-CGA-CHA
37	c	524	DGA	CBB-CAB-CB9-CB8
38	L	101	LHG	C26-C27-C28-C29
38	G	624	LHG	C13-C14-C15-C16
38	d	408	LHG	C28-C29-C30-C31
38	d	408	LHG	C30-C31-C32-C33
38	l	101	LHG	C11-C12-C13-C14
45	i	101	4RF	C05-C06-C07-C08
28	Y	614	CLA	O1A-CGA-O2A-C1
36	S	626	3PH	C2B-C2C-C2D-C2E
37	b	625	DGA	CB7-CB8-CB9-CAB
38	D	408	LHG	C33-C34-C35-C36
51	Y	626	PTY	C19-C20-C21-C22
31	b	621	SQD	C11-C10-C9-C8
36	T	101	3PH	C2B-C2C-C2D-C2E
37	c	524	DGA	CA6-CA7-CA8-CA9
37	j	101	DGA	CB7-CB8-CB9-CAB

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Mol	Chain	Res	Type	Atoms
38	S	624	LHG	C13-C14-C15-C16
45	K	101	4RF	C24-C25-C26-C27
28	A	410	CLA	C3-C5-C6-C7
28	b	602	CLA	C3-C5-C6-C7
31	b	626	SQD	C7-C8-C9-C10
32	w	201	LMG	C28-C29-C30-C31
31	B	626	SQD	C2-C1-O6-C44
32	B	622	LMG	C2-C1-O1-C7
35	C	519	DGD	C2E-C1E-O5D-C6D
49	G	623	NEX	C28-C29-C30-C31
49	G	623	NEX	C32-C33-C34-C35
49	Y	623	NEX	C28-C29-C30-C31
39	c	527	LMK	O7-C8-C9-O8
28	C	508	CLA	CBA-CGA-O2A-C1
28	b	612	CLA	CBA-CGA-O2A-C1
35	C	518	DGD	C3A-C4A-C5A-C6A
36	B	624	3PH	C2B-C2C-C2D-C2E
38	N	624	LHG	C13-C14-C15-C16
38	G	624	LHG	C11-C10-C9-C8
45	K	101	4RF	C26-C27-C28-C29
45	K	101	4RF	C46-C47-C48-C49
28	C	507	CLA	C13-C15-C16-C17
28	Y	613	CLA	C10-C11-C12-C13
28	a	405	CLA	C5-C6-C7-C8
28	G	603	CLA	O1A-CGA-O2A-C1
28	b	604	CLA	O1A-CGA-O2A-C1
28	Y	610	CLA	C16-C17-C18-C20
36	b	624	3PH	C28-C29-C2A-C2B
38	L	101	LHG	C11-C10-C9-C8
38	c	525	LHG	C24-C25-C26-C27
45	I	102	4RF	C07-C08-C09-C10
45	K	101	4RF	C44-C45-C46-C47
28	c	504	CLA	C2-C3-C5-C6
28	B	602	CLA	C11-C12-C13-C14
28	B	605	CLA	C11-C10-C8-C9
28	C	503	CLA	C6-C7-C8-C9
28	C	513	CLA	C11-C12-C13-C14
28	a	406	CLA	C11-C12-C13-C14
28	d	403	CLA	C11-C12-C13-C14
46	G	601	CHL	C11-C12-C13-C14
46	G	601	CHL	C14-C13-C15-C16
46	G	607	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
38	D	408	LHG	C23-C24-C25-C26
38	L	101	LHG	C23-C24-C25-C26
38	N	624	LHG	C23-C24-C25-C26
38	c	525	LHG	C7-C8-C9-C10
31	c	526	SQD	C17-C18-C19-C20
32	C	523	LMG	C18-C19-C20-C21
36	B	624	3PH	C24-C25-C26-C27
36	B	624	3PH	C3D-C3E-C3F-C3G
37	J	101	DGA	CB5-CB6-CB7-CB8
37	b	625	DGA	CA9-CAA-CBA-CCA
38	S	624	LHG	C11-C12-C13-C14
38	l	101	LHG	C28-C29-C30-C31
45	I	102	4RF	C32-C33-C34-C35
28	G	602	CLA	C10-C11-C12-C13
28	b	614	CLA	C15-C16-C17-C18
28	c	506	CLA	C10-C11-C12-C13
28	Y	608	CLA	C2A-CAA-CBA-CGA
28	a	406	CLA	C2A-CAA-CBA-CGA
28	c	501	CLA	C2A-CAA-CBA-CGA
46	N	608	CHL	C2A-CAA-CBA-CGA
30	a	411	BCR	C11-C12-C13-C35
30	d	404	BCR	C37-C22-C23-C24
34	B	620	C7Z	C7-C8-C9-C19
32	H	102	LMG	C13-C14-C15-C16
35	c	520	DGD	C5A-C6A-C7A-C8A
36	B	624	3PH	C25-C26-C27-C28
37	c	524	DGA	CAB-CBB-CCB-CDB
38	N	624	LHG	C14-C15-C16-C17
38	l	101	LHG	C26-C27-C28-C29
45	K	101	4RF	C45-C46-C47-C48
45	i	101	4RF	C09-C10-C11-C12
51	Y	626	PTY	C39-C40-C41-C42
38	C	525	LHG	O1-C1-C2-C3
38	D	409	LHG	O1-C1-C2-C3
38	D	410	LHG	O1-C1-C2-C3
38	L	101	LHG	O1-C1-C2-C3
38	G	624	LHG	O1-C1-C2-C3
38	Y	624	LHG	O1-C1-C2-C3
38	c	525	LHG	O1-C1-C2-C3
38	d	409	LHG	O1-C1-C2-C3
30	b	619	BCR	C17-C18-C19-C20
30	d	404	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
34	B	620	C7Z	C7-C8-C9-C10
28	B	617	CLA	C3-C5-C6-C7
28	Y	611	CLA	C3-C5-C6-C7
32	C	521	LMG	O9-C10-O7-C8
38	C	525	LHG	O9-C7-O7-C5
28	C	503	CLA	C8-C10-C11-C12
28	d	402	CLA	C15-C16-C17-C18
31	B	626	SQD	C8-C7-O47-C45
32	C	521	LMG	C11-C10-O7-C8
38	C	525	LHG	C8-C7-O7-C5
31	B	626	SQD	C16-C17-C18-C19
32	c	521	LMG	C11-C12-C13-C14
33	Y	625	SPH	C14-C15-C16-C17
38	D	409	LHG	C11-C12-C13-C14
38	S	624	LHG	C23-C24-C25-C26
31	A	412	SQD	C11-C12-C13-C14
31	b	621	SQD	C9-C10-C11-C12
32	w	201	LMG	C36-C37-C38-C39
36	t	101	3PH	C2B-C2C-C2D-C2E
37	B	625	DGA	CA4-CA5-CA6-CA7
37	J	101	DGA	CA4-CA5-CA6-CA7
37	c	524	DGA	CB3-CB4-CB5-CB6
38	C	525	LHG	C28-C29-C30-C31
38	D	408	LHG	C11-C12-C13-C14
38	Y	624	LHG	C16-C17-C18-C19
38	c	525	LHG	C13-C14-C15-C16
38	c	525	LHG	C26-C27-C28-C29
45	i	101	4RF	C43-C44-C45-C46
32	H	102	LMG	O6-C5-C6-O5
28	C	509	CLA	C16-C17-C18-C20
28	D	402	CLA	C16-C17-C18-C20
28	G	602	CLA	C16-C17-C18-C19
28	G	602	CLA	C16-C17-C18-C20
28	G	611	CLA	C16-C17-C18-C19
28	G	611	CLA	C16-C17-C18-C20
28	G	613	CLA	C16-C17-C18-C19
28	Y	613	CLA	C16-C17-C18-C19
28	c	501	CLA	C16-C17-C18-C19
28	c	501	CLA	C16-C17-C18-C20
28	c	507	CLA	C16-C17-C18-C19
28	c	507	CLA	C16-C17-C18-C20
31	M	101	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
31	c	526	SQD	O5-C1-O6-C44
28	c	505	CLA	C5-C6-C7-C8
28	c	506	CLA	C15-C16-C17-C18
31	B	626	SQD	C28-C29-C30-C31
36	S	626	3PH	C24-C25-C26-C27
36	t	101	3PH	C27-C28-C29-C2A
37	J	101	DGA	CA2-CA3-CA4-CA5
37	j	101	DGA	CB6-CB7-CB8-CB9
38	Y	624	LHG	C28-C29-C30-C31
38	Y	624	LHG	C31-C32-C33-C34
38	c	525	LHG	C29-C30-C31-C32
45	K	101	4RF	C10-C11-C12-C13
45	k	101	4RF	C27-C28-C29-C30
33	Y	625	SPH	C11-C10-C9-C8
33	a	414	SPH	C7-C8-C9-C10
36	b	624	3PH	C3E-C3F-C3G-C3H
37	B	625	DGA	CA5-CA6-CA7-CA8
38	Y	624	LHG	C29-C30-C31-C32
38	d	409	LHG	C28-C29-C30-C31
45	K	101	4RF	C27-C28-C29-C30
45	i	101	4RF	C22-C24-C25-C26
28	B	602	CLA	C10-C11-C12-C13
28	c	508	CLA	C10-C11-C12-C13
28	C	510	CLA	O1A-CGA-O2A-C1
28	a	405	CLA	O1A-CGA-O2A-C1
33	A	414	SPH	C12-C13-C14-C15
38	l	101	LHG	C13-C14-C15-C16
28	C	504	CLA	CBA-CGA-O2A-C1
28	S	603	CLA	CBA-CGA-O2A-C1
28	Y	610	CLA	CBA-CGA-O2A-C1
31	A	412	SQD	C24-C23-O48-C46
32	d	411	LMG	C19-C20-C21-C22
36	S	626	3PH	C29-C2A-C2B-C2C
37	c	524	DGA	CA8-CA9-CAA-CBA
51	Y	626	PTY	C36-C37-C38-C39
28	B	609	CLA	C3A-C2A-CAA-CBA
28	B	613	CLA	C3A-C2A-CAA-CBA
28	C	507	CLA	C3A-C2A-CAA-CBA
28	C	512	CLA	C3A-C2A-CAA-CBA
28	C	513	CLA	C3A-C2A-CAA-CBA
28	N	603	CLA	C3A-C2A-CAA-CBA
28	N	614	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	G	603	CLA	C3A-C2A-CAA-CBA
28	S	605	CLA	C3A-C2A-CAA-CBA
28	Y	603	CLA	C3A-C2A-CAA-CBA
28	c	507	CLA	C3A-C2A-CAA-CBA
28	c	513	CLA	C3A-C2A-CAA-CBA
29	A	408	PHO	C3A-C2A-CAA-CBA
46	G	606	CHL	C3A-C2A-CAA-CBA
46	G	607	CHL	C3A-C2A-CAA-CBA
30	C	515	BCR	C9-C10-C11-C12
37	b	625	DGA	CA4-CA5-CA6-CA7
37	b	625	DGA	CDB-CEB-CFB-CGB
37	c	524	DGA	CB9-CAB-CBB-CCB
38	D	409	LHG	C10-C11-C12-C13
28	C	501	CLA	C16-C17-C18-C20
28	C	513	CLA	C16-C17-C18-C20
32	h	102	LMG	C12-C13-C14-C15
33	Y	625	SPH	C6-C7-C8-C9
37	b	625	DGA	CA6-CA7-CA8-CA9
38	D	409	LHG	C25-C26-C27-C28
38	D	409	LHG	C28-C29-C30-C31
38	Y	624	LHG	C11-C10-C9-C8
38	l	101	LHG	C11-C10-C9-C8
45	I	102	4RF	C44-C45-C46-C47
32	b	622	LMG	C7-C8-C9-O8
38	Y	624	LHG	C4-C5-C6-O8
31	B	626	SQD	O49-C7-O47-C45
38	d	408	LHG	C11-C12-C13-C14
28	C	511	CLA	C3-C5-C6-C7
38	L	101	LHG	C9-C10-C11-C12
38	G	624	LHG	C28-C29-C30-C31
45	k	101	4RF	C34-C35-C36-C37
51	Y	626	PTY	C22-C23-C24-C25
29	A	408	PHO	C4-C3-C5-C6
29	a	408	PHO	C4-C3-C5-C6
46	Y	607	CHL	C4-C3-C5-C6
29	A	408	PHO	C2-C3-C5-C6
29	a	408	PHO	C2-C3-C5-C6
46	Y	607	CHL	C2-C3-C5-C6
36	B	624	3PH	C22-C21-O21-C2
35	C	519	DGD	C4B-C5B-C6B-C7B
37	c	524	DGA	CB5-CB6-CB7-CB8
38	D	408	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
38	D	409	LHG	O1-C1-C2-O2
38	G	624	LHG	O1-C1-C2-O2
38	S	624	LHG	O1-C1-C2-O2
38	c	525	LHG	O1-C1-C2-O2
38	d	408	LHG	O1-C1-C2-O2
38	d	409	LHG	O1-C1-C2-O2
38	d	410	LHG	O1-C1-C2-O2
39	C	527	LMK	O9-C10-C11-C12
44	I	101	GOL	O2-C2-C3-O3
28	Y	610	CLA	C5-C6-C7-C8
32	D	411	LMG	C19-C20-C21-C22
36	T	101	3PH	C24-C25-C26-C27
36	T	101	3PH	C25-C26-C27-C28
38	N	624	LHG	C28-C29-C30-C31
38	c	525	LHG	C25-C26-C27-C28
38	d	409	LHG	C13-C14-C15-C16
28	B	602	CLA	O1A-CGA-O2A-C1
38	d	408	LHG	O10-C23-O8-C6
28	b	602	CLA	C16-C17-C18-C19
28	c	513	CLA	C16-C17-C18-C19
28	d	402	CLA	C16-C17-C18-C19
28	Y	612	CLA	C5-C6-C7-C8
28	b	603	CLA	C8-C10-C11-C12
37	B	625	DGA	CA3-CA4-CA5-CA6
37	B	625	DGA	CB3-CB4-CB5-CB6
51	Y	626	PTY	C40-C41-C42-C43
28	C	508	CLA	C3-C5-C6-C7
35	c	518	DGD	O6E-C5E-C6E-O5E
31	b	621	SQD	C24-C23-O48-C46
37	C	524	DGA	CA9-CAA-CBA-CCA
38	d	408	LHG	C13-C14-C15-C16
38	d	408	LHG	C25-C26-C27-C28
28	Y	611	CLA	C13-C15-C16-C17
38	D	410	LHG	C1-C2-C3-O3
31	B	621	SQD	C13-C14-C15-C16
31	m	101	SQD	C27-C28-C29-C30
35	C	519	DGD	C3A-C4A-C5A-C6A
38	c	525	LHG	C28-C29-C30-C31
45	k	101	4RF	C28-C29-C30-C31
36	B	624	3PH	O22-C21-O21-C2
28	B	606	CLA	C2-C1-O2A-CGA
28	B	616	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
28	B	617	CLA	C2-C1-O2A-CGA
28	C	502	CLA	C2-C1-O2A-CGA
28	C	503	CLA	C2-C1-O2A-CGA
28	C	507	CLA	C2-C1-O2A-CGA
28	C	510	CLA	C2-C1-O2A-CGA
28	N	613	CLA	C2-C1-O2A-CGA
28	S	614	CLA	C2-C1-O2A-CGA
28	b	611	CLA	C2-C1-O2A-CGA
28	b	617	CLA	C2-C1-O2A-CGA
28	c	502	CLA	C2-C1-O2A-CGA
28	c	503	CLA	C2-C1-O2A-CGA
28	c	504	CLA	C2-C1-O2A-CGA
28	c	510	CLA	C2-C1-O2A-CGA
37	C	524	DGA	CA6-CA7-CA8-CA9
38	D	408	LHG	C26-C27-C28-C29
38	d	409	LHG	C34-C35-C36-C37
45	K	101	4RF	C11-C12-C13-C14
28	D	403	CLA	C8-C10-C11-C12
31	A	412	SQD	O10-C23-O48-C46
38	L	101	LHG	C16-C17-C18-C19
38	N	624	LHG	C25-C26-C27-C28
38	l	101	LHG	C9-C10-C11-C12
28	S	604	CLA	C6-C7-C8-C9
28	b	605	CLA	C16-C17-C18-C19
37	c	524	DGA	CA1-CA2-CA3-CA4
45	k	101	4RF	C13-C14-C15-C16
30	A	411	BCR	C23-C24-C25-C26
30	A	411	BCR	C23-C24-C25-C30
30	C	514	BCR	C1-C6-C7-C8
30	C	514	BCR	C5-C6-C7-C8
30	C	515	BCR	C1-C6-C7-C8
30	C	515	BCR	C5-C6-C7-C8
30	C	516	BCR	C23-C24-C25-C26
30	C	517	BCR	C23-C24-C25-C30
30	D	404	BCR	C1-C6-C7-C8
30	D	404	BCR	C5-C6-C7-C8
30	a	411	BCR	C23-C24-C25-C26
30	a	411	BCR	C23-C24-C25-C30
30	b	619	BCR	C23-C24-C25-C26
30	c	514	BCR	C1-C6-C7-C8
30	c	514	BCR	C5-C6-C7-C8
30	c	515	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	c	515	BCR	C23-C24-C25-C30
30	c	516	BCR	C1-C6-C7-C8
30	c	516	BCR	C5-C6-C7-C8
30	c	516	BCR	C23-C24-C25-C26
30	c	516	BCR	C23-C24-C25-C30
30	d	404	BCR	C1-C6-C7-C8
30	d	404	BCR	C5-C6-C7-C8
34	B	620	C7Z	C1-C6-C7-C8
34	B	620	C7Z	C5-C6-C7-C8
34	B	620	C7Z	C21-C26-C27-C28
34	B	620	C7Z	C25-C26-C27-C28
34	b	620	C7Z	C1-C6-C7-C8
34	b	620	C7Z	C5-C6-C7-C8
34	b	620	C7Z	C25-C26-C27-C28
43	H	101	RRX	C5-C6-C7-C8
47	N	620	LUT	C5-C6-C7-C8
38	D	410	LHG	C24-C23-O8-C6
38	c	525	LHG	C24-C23-O8-C6
45	k	101	4RF	C43-C41-O40-C39
28	C	501	CLA	C5-C6-C7-C8
28	C	511	CLA	C8-C10-C11-C12
28	C	513	CLA	C15-C16-C17-C18
28	N	604	CLA	C13-C15-C16-C17
28	S	611	CLA	C15-C16-C17-C18
28	Y	602	CLA	C5-C6-C7-C8
37	b	625	DGA	CB9-CAB-CBB-CCB
38	d	410	LHG	C33-C34-C35-C36
45	k	101	4RF	C24-C25-C26-C27
28	C	508	CLA	O1A-CGA-O2A-C1
28	S	603	CLA	O1A-CGA-O2A-C1
36	t	101	3PH	C22-C23-C24-C25
38	C	525	LHG	C26-C27-C28-C29
41	d	405	PL9	C47-C48-C49-C50
28	B	614	CLA	C8-C10-C11-C12
28	B	616	CLA	C10-C11-C12-C13
37	C	524	DGA	CB9-CAB-CBB-CCB
28	N	603	CLA	C4-C3-C5-C6
28	c	510	CLA	C4-C3-C5-C6
41	D	405	PL9	C40-C39-C41-C42
28	B	603	CLA	C12-C13-C15-C16
28	B	605	CLA	C6-C7-C8-C10
28	B	605	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
28	B	613	CLA	C12-C13-C15-C16
28	B	615	CLA	C6-C7-C8-C10
28	C	501	CLA	C2-C3-C5-C6
28	C	503	CLA	C6-C7-C8-C10
28	C	505	CLA	C6-C7-C8-C10
28	C	513	CLA	C11-C12-C13-C15
28	N	613	CLA	C2-C3-C5-C6
28	S	603	CLA	C11-C10-C8-C7
28	a	406	CLA	C11-C12-C13-C15
28	b	605	CLA	C6-C7-C8-C10
28	b	608	CLA	C11-C12-C13-C15
28	b	610	CLA	C11-C12-C13-C15
28	c	509	CLA	C12-C13-C15-C16
28	c	510	CLA	C2-C3-C5-C6
28	c	511	CLA	C11-C12-C13-C15
28	d	402	CLA	C6-C7-C8-C10
28	d	402	CLA	C11-C12-C13-C15
28	d	403	CLA	C11-C10-C8-C7
41	D	405	PL9	C38-C39-C41-C42
41	d	405	PL9	C13-C14-C16-C17
28	C	504	CLA	O1A-CGA-O2A-C1
28	Y	610	CLA	O1A-CGA-O2A-C1
28	b	612	CLA	O1A-CGA-O2A-C1
36	T	101	3PH	C37-C38-C39-C3A
38	N	624	LHG	C11-C12-C13-C14
28	B	617	CLA	C10-C11-C12-C13
28	C	507	CLA	C5-C6-C7-C8
28	S	611	CLA	C10-C11-C12-C13
28	b	616	CLA	C8-C10-C11-C12
28	c	503	CLA	C8-C10-C11-C12
38	l	101	LHG	C5-C6-O8-C23
30	B	618	BCR	C13-C14-C15-C16
30	C	514	BCR	C15-C16-C17-C18
30	C	516	BCR	C9-C10-C11-C12
30	C	517	BCR	C9-C10-C11-C12
28	N	610	CLA	C16-C17-C18-C20
38	D	410	LHG	O9-C7-O7-C5
38	Y	624	LHG	O9-C7-O7-C5
36	b	624	3PH	C21-C22-C23-C24
28	A	410	CLA	CBA-CGA-O2A-C1
28	G	610	CLA	CBA-CGA-O2A-C1
38	C	525	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
28	b	604	CLA	C2A-CAA-CBA-CGA
28	A	406	CLA	C13-C15-C16-C17
28	b	607	CLA	C5-C6-C7-C8
36	t	101	3PH	C3C-C3D-C3E-C3F
37	B	625	DGA	CB5-CB6-CB7-CB8
38	C	525	LHG	C25-C26-C27-C28
38	D	409	LHG	C34-C35-C36-C37
38	c	525	LHG	C30-C31-C32-C33
35	c	519	DGD	C1B-C2B-C3B-C4B
28	B	602	CLA	O1D-CGD-O2D-CED
28	C	509	CLA	C10-C11-C12-C13
28	Y	604	CLA	C10-C11-C12-C13
28	b	614	CLA	C8-C10-C11-C12
32	D	411	LMG	C12-C13-C14-C15
35	c	519	DGD	C6B-C7B-C8B-C9B
36	B	624	3PH	C22-C23-C24-C25
37	b	625	DGA	CB5-CB6-CB7-CB8
38	L	101	LHG	C28-C29-C30-C31
28	b	610	CLA	C3-C5-C6-C7
38	d	409	LHG	C10-C11-C12-C13
32	D	411	LMG	O6-C5-C6-O5
35	C	518	DGD	C2A-C1A-O1G-C1G
28	C	510	CLA	C16-C17-C18-C20
35	c	519	DGD	O6E-C1E-O5D-C6D
28	B	609	CLA	C13-C15-C16-C17
28	b	611	CLA	C13-C15-C16-C17
28	b	617	CLA	C5-C6-C7-C8
32	C	521	LMG	C14-C15-C16-C17
35	C	519	DGD	CCB-CDB-CEB-CFB
37	B	625	DGA	CA8-CA9-CAA-CBA
38	D	410	LHG	C33-C34-C35-C36
45	k	101	4RF	C08-C09-C10-C11
51	Y	626	PTY	C23-C24-C25-C26
35	C	519	DGD	C1B-C2B-C3B-C4B
36	B	624	3PH	C21-C22-C23-C24
37	B	625	DGA	CB1-CB2-CB3-CB4
37	b	625	DGA	CB1-CB2-CB3-CB4
38	G	624	LHG	C23-C24-C25-C26
32	D	411	LMG	C11-C10-O7-C8
32	c	521	LMG	C11-C10-O7-C8
38	D	410	LHG	C8-C7-O7-C5
38	Y	624	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
37	B	625	DGA	CB7-CB8-CB9-CAB
38	l	101	LHG	C25-C26-C27-C28
45	k	101	4RF	C43-C44-C45-C46
28	B	606	CLA	C8-C10-C11-C12
28	G	610	CLA	C10-C11-C12-C13
28	b	617	CLA	C15-C16-C17-C18
28	c	501	CLA	C8-C10-C11-C12
31	C	526	SQD	C9-C10-C11-C12
35	c	518	DGD	C3A-C4A-C5A-C6A
38	Y	624	LHG	C30-C31-C32-C33
39	c	527	LMK	C2-C3-C4-O2
28	B	607	CLA	C3-C5-C6-C7
28	B	609	CLA	C3-C5-C6-C7
38	G	624	LHG	C9-C10-C11-C12
38	d	408	LHG	C29-C30-C31-C32
38	l	101	LHG	C31-C32-C33-C34
39	C	527	LMK	C12-C13-C14-C15
38	Y	624	LHG	O7-C5-C6-O8
38	d	410	LHG	O7-C5-C6-O8
45	I	102	4RF	O21-C20-C39-O40
38	d	408	LHG	C24-C25-C26-C27
45	K	101	4RF	C32-C33-C34-C35
45	k	101	4RF	C48-C49-C50-C51
28	Y	610	CLA	C16-C17-C18-C19
46	S	608	CHL	C11-C12-C13-C14
38	L	101	LHG	C10-C11-C12-C13
32	c	521	LMG	O6-C5-C6-O5
35	C	519	DGD	O6E-C5E-C6E-O5E
28	B	604	CLA	C5-C6-C7-C8
28	B	612	CLA	C8-C10-C11-C12
28	S	602	CLA	C4-C3-C5-C6
41	D	405	PL9	C15-C14-C16-C17
36	T	101	3PH	C31-C32-C33-C34
38	Y	624	LHG	C23-C24-C25-C26
28	N	603	CLA	C2-C3-C5-C6
28	Y	611	CLA	C2-C3-C5-C6
46	N	601	CHL	C2-C3-C5-C6
28	A	406	CLA	C11-C12-C13-C14
28	B	613	CLA	C14-C13-C15-C16
28	B	615	CLA	C6-C7-C8-C9
28	B	616	CLA	C14-C13-C15-C16
28	C	505	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	C	512	CLA	C14-C13-C15-C16
28	N	604	CLA	C6-C7-C8-C9
28	N	610	CLA	C6-C7-C8-C9
28	G	603	CLA	C6-C7-C8-C9
28	G	611	CLA	C6-C7-C8-C9
28	S	603	CLA	C11-C10-C8-C9
28	b	602	CLA	C6-C7-C8-C9
28	b	602	CLA	C11-C10-C8-C9
28	b	604	CLA	C11-C12-C13-C14
28	b	606	CLA	C11-C10-C8-C9
28	b	613	CLA	C14-C13-C15-C16
28	c	509	CLA	C14-C13-C15-C16
28	c	510	CLA	C14-C13-C15-C16
28	c	511	CLA	C11-C12-C13-C14
28	d	402	CLA	C11-C12-C13-C14
28	d	403	CLA	C11-C10-C8-C9
46	N	605	CHL	C11-C10-C8-C9
35	c	519	DGD	O6E-C5E-C6E-O5E
28	A	410	CLA	O1A-CGA-O2A-C1
31	c	526	SQD	C9-C10-C11-C12
36	t	101	3PH	C37-C38-C39-C3A
37	j	101	DGA	CA6-CA7-CA8-CA9
45	K	101	4RF	C08-C09-C10-C11
36	B	624	3PH	C3B-C3C-C3D-C3E
37	c	524	DGA	CDB-CEB-CFB-CGB
38	D	408	LHG	C29-C30-C31-C32
38	L	101	LHG	C25-C26-C27-C28
45	K	101	4RF	C09-C10-C11-C12
32	h	102	LMG	O6-C5-C6-O5
35	b	623	DGD	O6E-C5E-C6E-O5E
28	S	614	CLA	CBA-CGA-O2A-C1
28	c	502	CLA	C13-C15-C16-C17
37	b	625	DGA	CA8-CA9-CAA-CBA
45	i	101	4RF	C10-C11-C12-C13
30	C	514	BCR	C17-C18-C19-C20
30	C	514	BCR	C21-C22-C23-C24
30	C	516	BCR	C17-C18-C19-C20
34	b	620	C7Z	C31-C32-C33-C34
45	k	101	4RF	O42-C41-O40-C39
28	A	407	CLA	C1A-C2A-CAA-CBA
28	B	602	CLA	C1A-C2A-CAA-CBA
28	B	605	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	B	607	CLA	C1A-C2A-CAA-CBA
28	C	501	CLA	C1A-C2A-CAA-CBA
28	C	503	CLA	C1A-C2A-CAA-CBA
28	C	507	CLA	C1A-C2A-CAA-CBA
28	C	511	CLA	C1A-C2A-CAA-CBA
28	D	402	CLA	C1A-C2A-CAA-CBA
28	N	603	CLA	C1A-C2A-CAA-CBA
28	G	603	CLA	C1A-C2A-CAA-CBA
28	G	604	CLA	C1A-C2A-CAA-CBA
28	G	610	CLA	C1A-C2A-CAA-CBA
28	G	614	CLA	C1A-C2A-CAA-CBA
28	S	602	CLA	C1A-C2A-CAA-CBA
28	S	604	CLA	C1A-C2A-CAA-CBA
28	S	609	CLA	C1A-C2A-CAA-CBA
28	S	617	CLA	C1A-C2A-CAA-CBA
28	Y	603	CLA	C1A-C2A-CAA-CBA
28	Y	608	CLA	C1A-C2A-CAA-CBA
28	Y	610	CLA	C1A-C2A-CAA-CBA
28	Y	611	CLA	C1A-C2A-CAA-CBA
28	Y	614	CLA	C1A-C2A-CAA-CBA
28	a	406	CLA	C1A-C2A-CAA-CBA
28	a	407	CLA	C1A-C2A-CAA-CBA
28	b	604	CLA	C1A-C2A-CAA-CBA
28	c	501	CLA	C1A-C2A-CAA-CBA
28	c	503	CLA	C1A-C2A-CAA-CBA
28	c	507	CLA	C1A-C2A-CAA-CBA
28	c	512	CLA	C1A-C2A-CAA-CBA
46	N	607	CHL	C1A-C2A-CAA-CBA
46	G	606	CHL	C1A-C2A-CAA-CBA
28	G	610	CLA	C16-C17-C18-C19
28	Y	613	CLA	C16-C17-C18-C20
28	b	605	CLA	C16-C17-C18-C20
28	b	609	CLA	C16-C17-C18-C19
28	c	513	CLA	C16-C17-C18-C20
32	D	411	LMG	O9-C10-O7-C8
32	c	521	LMG	O9-C10-O7-C8
37	C	524	DGA	OB1-CB1-OG2-CG2
37	C	524	DGA	CB2-CB1-OG2-CG2
38	c	525	LHG	C8-C7-O7-C5
32	H	102	LMG	C37-C38-C39-C40
36	S	626	3PH	C22-C23-C24-C25
37	b	625	DGA	CA5-CA6-CA7-CA8

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Mol	Chain	Res	Type	Atoms
38	d	408	LHG	C33-C34-C35-C36
43	h	101	RRX	C9-C10-C11-C12
28	b	602	CLA	C13-C15-C16-C17
28	b	607	CLA	C8-C10-C11-C12
38	L	101	LHG	C13-C14-C15-C16
28	C	507	CLA	C3-C5-C6-C7
28	S	602	CLA	C3-C5-C6-C7
45	k	101	4RF	C45-C46-C47-C48
38	c	525	LHG	O10-C23-O8-C6
28	D	403	CLA	C13-C15-C16-C17
28	Y	613	CLA	C8-C10-C11-C12
28	B	612	CLA	CBA-CGA-O2A-C1
36	B	624	3PH	O11-C1-C2-C3
36	t	101	3PH	O11-C1-C2-C3
38	N	624	LHG	O6-C4-C5-C6
38	G	624	LHG	O6-C4-C5-C6
38	d	408	LHG	O6-C4-C5-C6
38	d	409	LHG	O6-C4-C5-C6
51	Y	627	PTY	O14-C5-C6-C1
38	d	408	LHG	C7-C8-C9-C10
32	C	523	LMG	C16-C17-C18-C19
28	C	501	CLA	C16-C17-C18-C19
28	C	507	CLA	C16-C17-C18-C19
28	S	604	CLA	C6-C7-C8-C10
28	c	511	CLA	C16-C17-C18-C20
38	D	410	LHG	C25-C26-C27-C28
38	Y	624	LHG	C11-C12-C13-C14
38	l	101	LHG	C30-C31-C32-C33
28	b	608	CLA	C15-C16-C17-C18
31	a	412	SQD	C26-C27-C28-C29
38	D	409	LHG	C15-C16-C17-C18
45	I	102	4RF	C51-C52-C53-C54
28	N	613	CLA	C4-C3-C5-C6
31	b	621	SQD	C24-C25-C26-C27
37	C	524	DGA	CCA-CDA-CEA-CFA
28	B	603	CLA	C5-C6-C7-C8
28	B	616	CLA	C13-C15-C16-C17
28	Y	612	CLA	C13-C15-C16-C17
38	d	409	LHG	C11-C12-C13-C14
38	d	410	LHG	C28-C29-C30-C31
45	i	101	4RF	C33-C34-C35-C36
31	b	621	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
38	D	410	LHG	O10-C23-O8-C6
36	b	624	3PH	C2E-C2F-C2G-C2H
36	t	101	3PH	C25-C26-C27-C28
37	b	625	DGA	CA2-CA3-CA4-CA5
31	A	412	SQD	O6-C44-C45-C46
31	B	626	SQD	C44-C45-C46-O48
31	C	526	SQD	C44-C45-C46-O48
31	M	101	SQD	C44-C45-C46-O48
31	a	412	SQD	O6-C44-C45-C46
32	a	413	LMG	C7-C8-C9-O8
32	w	201	LMG	O1-C7-C8-C9
35	C	520	DGD	CCB-CDB-CEB-CFB
35	b	623	DGD	O1G-C1G-C2G-C3G
36	S	626	3PH	C1-C2-C3-O31
37	j	101	DGA	OG1-CG1-CG2-CG3
38	L	101	LHG	C4-C5-C6-O8
38	N	624	LHG	C15-C16-C17-C18
38	S	624	LHG	C4-C5-C6-O8
38	d	410	LHG	C4-C5-C6-O8
38	l	101	LHG	C4-C5-C6-O8
39	C	527	LMK	O1-C7-C8-C9
35	c	520	DGD	C2A-C1A-O1G-C1G
28	B	617	CLA	C8-C10-C11-C12
32	c	521	LMG	C19-C20-C21-C22
37	b	625	DGA	CBB-CAB-CB9-CB8
38	d	409	LHG	C25-C26-C27-C28
45	I	102	4RF	C09-C10-C11-C12
32	W	201	LMG	C8-C7-O1-C1
35	C	519	DGD	C2G-C3G-O3G-C1D
35	c	519	DGD	C2G-C3G-O3G-C1D
31	a	412	SQD	C31-C32-C33-C34
37	C	524	DGA	CA8-CA9-CAA-CBA
38	d	410	LHG	C29-C30-C31-C32
28	A	405	CLA	C5-C6-C7-C8
28	C	512	CLA	C15-C16-C17-C18
28	Y	611	CLA	C5-C6-C7-C8
28	b	603	CLA	C13-C15-C16-C17
38	L	101	LHG	C31-C32-C33-C34
38	N	624	LHG	O8-C23-C24-C25
35	C	518	DGD	O1A-C1A-O1G-C1G
35	c	519	DGD	CAB-CBB-CCB-CDB
35	c	519	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
38	N	624	LHG	O1-C1-C2-O2
38	Y	624	LHG	O1-C1-C2-O2
28	D	403	CLA	C10-C11-C12-C13
28	G	610	CLA	O1A-CGA-O2A-C1
38	D	409	LHG	C29-C30-C31-C32
38	D	409	LHG	C30-C31-C32-C33
38	S	624	LHG	C28-C29-C30-C31
50	S	625	LPX	C10-C11-C12-C13
37	C	524	DGA	CB4-CB5-CB6-CB7
28	B	615	CLA	C5-C6-C7-C8
30	c	516	BCR	C11-C10-C9-C34
32	C	521	LMG	O6-C5-C6-O5
35	B	623	DGD	O6E-C5E-C6E-O5E
35	C	518	DGD	O6E-C5E-C6E-O5E
28	b	602	CLA	C4-C3-C5-C6
45	i	101	4RF	C06-C07-C08-C09
38	S	624	LHG	C7-C8-C9-C10
45	K	101	4RF	C41-C43-C44-C45
28	B	617	CLA	CBA-CGA-O2A-C1
35	c	519	DGD	C2A-C1A-O1G-C1G
39	C	527	LMK	C11-C12-C13-C14
28	N	610	CLA	C13-C15-C16-C17
28	c	505	CLA	C8-C10-C11-C12
31	B	621	SQD	C46-C45-O47-C7
33	a	414	SPH	O3-C3-C4-C5
36	T	101	3PH	C3-C2-O21-C21
37	B	625	DGA	CG1-CG2-OG2-CB1
37	b	625	DGA	CG1-CG2-OG2-CB1
28	C	502	CLA	C2A-CAA-CBA-CGA
28	b	606	CLA	C2A-CAA-CBA-CGA
28	S	614	CLA	O1A-CGA-O2A-C1
28	c	507	CLA	C2-C1-O2A-CGA
29	a	409	PHO	C2-C1-O2A-CGA
36	b	624	3PH	C27-C28-C29-C2A
33	a	414	SPH	C12-C13-C14-C15
38	S	624	LHG	C31-C32-C33-C34
51	Y	626	PTY	C41-C42-C43-C44
36	T	101	3PH	C1-O11-P-O12
36	t	101	3PH	C36-C37-C38-C39
37	b	625	DGA	CCB-CDB-CEB-CFB
38	L	101	LHG	C11-C12-C13-C14
28	b	602	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	B	617	CLA	C16-C17-C18-C20
28	N	610	CLA	C16-C17-C18-C19
28	B	604	CLA	C15-C16-C17-C18
31	a	412	SQD	C25-C26-C27-C28
33	a	414	SPH	C14-C15-C16-C17
28	B	612	CLA	O1A-CGA-O2A-C1
28	A	406	CLA	C5-C6-C7-C8
28	b	610	CLA	C13-C15-C16-C17
28	b	615	CLA	C13-C15-C16-C17
31	M	101	SQD	C2-C1-O6-C44
35	c	519	DGD	C2E-C1E-O5D-C6D
31	A	412	SQD	O6-C44-C45-O47
36	S	626	3PH	O21-C2-C3-O31
37	j	101	DGA	OG1-CG1-CG2-OG2
51	Y	627	PTY	O4-C1-C6-O7
38	c	525	LHG	O9-C7-O7-C5
28	S	602	CLA	C5-C6-C7-C8
28	b	608	CLA	C8-C10-C11-C12
35	c	520	DGD	O1A-C1A-O1G-C1G
28	C	510	CLA	C16-C17-C18-C19
28	A	406	CLA	O1D-CGD-O2D-CED
31	b	626	SQD	C16-C17-C18-C19
38	Y	624	LHG	C34-C35-C36-C37
41	d	405	PL9	C15-C14-C16-C17
37	b	625	DGA	CB3-CB4-CB5-CB6
28	A	405	CLA	C12-C13-C15-C16
28	A	406	CLA	C11-C10-C8-C7
28	B	602	CLA	C11-C12-C13-C15
28	B	616	CLA	C12-C13-C15-C16
28	C	502	CLA	C11-C12-C13-C15
28	C	512	CLA	C12-C13-C15-C16
28	D	402	CLA	C11-C12-C13-C15
28	N	604	CLA	C6-C7-C8-C10
28	N	610	CLA	C6-C7-C8-C10
28	G	603	CLA	C6-C7-C8-C10
28	G	610	CLA	C12-C13-C15-C16
28	G	611	CLA	C6-C7-C8-C10
28	S	602	CLA	C6-C7-C8-C10
28	Y	611	CLA	C6-C7-C8-C10
28	b	602	CLA	C2-C3-C5-C6
28	b	602	CLA	C6-C7-C8-C10
28	b	602	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
28	b	602	CLA	C11-C12-C13-C15
28	b	609	CLA	C12-C13-C15-C16
28	b	612	CLA	C11-C10-C8-C7
28	b	613	CLA	C12-C13-C15-C16
28	b	616	CLA	C11-C10-C8-C7
28	b	616	CLA	C11-C12-C13-C15
28	b	617	CLA	C6-C7-C8-C10
28	c	505	CLA	C12-C13-C15-C16
28	c	507	CLA	C12-C13-C15-C16
28	c	510	CLA	C11-C12-C13-C15
28	c	510	CLA	C12-C13-C15-C16
46	N	605	CHL	C11-C10-C8-C7
46	N	606	CHL	C11-C12-C13-C15
46	N	607	CHL	C11-C10-C8-C7
46	G	609	CHL	C11-C12-C13-C15
46	S	608	CHL	C11-C10-C8-C7
46	Y	606	CHL	C11-C12-C13-C15
46	Y	609	CHL	C12-C13-C15-C16
32	A	413	LMG	O7-C10-C11-C12
28	A	405	CLA	C14-C13-C15-C16
28	B	604	CLA	C11-C12-C13-C14
28	B	607	CLA	C11-C10-C8-C9
28	B	609	CLA	C11-C10-C8-C9
28	B	617	CLA	C6-C7-C8-C9
28	C	501	CLA	C14-C13-C15-C16
28	C	502	CLA	C11-C12-C13-C14
28	C	505	CLA	C14-C13-C15-C16
28	C	509	CLA	C14-C13-C15-C16
28	C	513	CLA	C6-C7-C8-C9
28	D	402	CLA	C11-C12-C13-C14
28	N	603	CLA	C14-C13-C15-C16
28	G	610	CLA	C14-C13-C15-C16
28	Y	612	CLA	C11-C10-C8-C9
28	b	602	CLA	C14-C13-C15-C16
28	b	617	CLA	C6-C7-C8-C9
28	c	504	CLA	C11-C10-C8-C9
28	c	505	CLA	C14-C13-C15-C16
28	c	507	CLA	C14-C13-C15-C16
28	c	513	CLA	C11-C12-C13-C14
46	N	606	CHL	C11-C10-C8-C9
46	N	607	CHL	C11-C10-C8-C9
46	N	607	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
46	G	609	CHL	C11-C12-C13-C14
46	S	608	CHL	C11-C10-C8-C9
46	Y	606	CHL	C6-C7-C8-C9
46	Y	607	CHL	C6-C7-C8-C9
46	Y	609	CHL	C14-C13-C15-C16
31	A	412	SQD	C33-C34-C35-C36
31	a	412	SQD	C10-C11-C12-C13
33	Y	625	SPH	C12-C13-C14-C15
37	c	524	DGA	CEB-CFB-CGB-CHB
38	C	525	LHG	C34-C35-C36-C37
38	L	101	LHG	C33-C34-C35-C36
38	Y	624	LHG	C33-C34-C35-C36
28	S	610	CLA	C2A-CAA-CBA-CGA
28	Y	610	CLA	C2A-CAA-CBA-CGA
32	C	523	LMG	C42-C43-C44-C45
38	L	101	LHG	C34-C35-C36-C37
45	i	101	4RF	C11-C12-C13-C14
30	C	516	BCR	C37-C22-C23-C24
30	c	517	BCR	C37-C22-C23-C24
32	c	521	LMG	C29-C30-C31-C32
33	A	414	SPH	C6-C7-C8-C9
30	B	619	BCR	C17-C18-C19-C20
30	c	515	BCR	C17-C18-C19-C20
30	d	404	BCR	C17-C18-C19-C20
28	C	512	CLA	C3-C5-C6-C7
28	B	615	CLA	C15-C16-C17-C18
28	a	410	CLA	C8-C10-C11-C12
28	b	610	CLA	C15-C16-C17-C18
28	c	510	CLA	C5-C6-C7-C8
36	b	624	3PH	C3F-C3G-C3H-C3I
36	t	101	3PH	C3D-C3E-C3F-C3G
38	N	624	LHG	C16-C17-C18-C19
38	d	409	LHG	C29-C30-C31-C32
35	c	519	DGD	O1A-C1A-O1G-C1G
28	c	513	CLA	CBA-CGA-O2A-C1
36	b	624	3PH	C2F-C2G-C2H-C2I
38	G	624	LHG	C11-C12-C13-C14
28	N	613	CLA	CAA-CBA-CGA-O2A
38	D	410	LHG	C24-C25-C26-C27
28	G	610	CLA	C16-C17-C18-C20
28	Y	603	CLA	C8-C10-C11-C12
36	b	624	3PH	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
38	C	525	LHG	O6-C4-C5-C6
38	D	410	LHG	O6-C4-C5-C6
35	C	520	DGD	C7A-C8A-C9A-CAA
35	C	519	DGD	C1A-C2A-C3A-C4A
35	c	519	DGD	C1A-C2A-C3A-C4A
38	D	408	LHG	C24-C25-C26-C27
38	d	408	LHG	C11-C10-C9-C8
28	B	615	CLA	C8-C10-C11-C12
28	G	602	CLA	C5-C6-C7-C8
45	K	101	4RF	C22-C24-C25-C26
45	K	101	4RF	C02-C03-C04-C05
28	N	603	CLA	C5-C6-C7-C8
28	c	507	CLA	C13-C15-C16-C17
45	k	101	4RF	C30-C31-C32-C33
36	B	624	3PH	C27-C28-C29-C2A
36	T	101	3PH	C2D-C2E-C2F-C2G
36	S	626	3PH	C36-C37-C38-C39
38	Y	624	LHG	C9-C10-C11-C12
38	d	408	LHG	C26-C27-C28-C29
31	b	621	SQD	O47-C7-C8-C9
37	b	625	DGA	CA1-CA2-CA3-CA4
31	B	626	SQD	C33-C34-C35-C36
36	T	101	3PH	C2-C1-O11-P
38	C	525	LHG	C2-C3-O3-P
38	D	410	LHG	C2-C3-O3-P
38	d	410	LHG	C2-C3-O3-P
28	N	613	CLA	C3A-C2A-CAA-CBA
29	a	408	PHO	C3A-C2A-CAA-CBA
38	c	525	LHG	C35-C36-C37-C38
45	k	101	4RF	C47-C48-C49-C50
30	c	517	BCR	C13-C14-C15-C16
34	B	620	C7Z	C29-C30-C31-C32
34	b	620	C7Z	C9-C10-C11-C12
43	h	101	RRX	C19-C20-C21-C22
47	Y	621	LUT	C29-C30-C31-C32
31	b	621	SQD	C14-C15-C16-C17
32	c	523	LMG	C18-C19-C20-C21
36	T	101	3PH	C36-C37-C38-C39
36	S	626	3PH	C2A-C2B-C2C-C2D
37	j	101	DGA	CA7-CA8-CA9-CAA
38	C	525	LHG	C13-C14-C15-C16
28	Y	614	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	B	622	LMG	C32-C33-C34-C35
36	t	101	3PH	C3A-C3B-C3C-C3D
37	J	101	DGA	CB3-CB4-CB5-CB6
37	b	625	DGA	CFB-CGB-CHB-CIB
28	A	410	CLA	C11-C12-C13-C15
28	G	603	CLA	C16-C17-C18-C20
45	K	101	4RF	C15-C16-O18-C19
38	d	408	LHG	C31-C32-C33-C34
28	d	403	CLA	C5-C6-C7-C8
31	a	412	SQD	C44-C45-C46-O48
35	B	623	DGD	O1G-C1G-C2G-C3G
36	t	101	3PH	C1-C2-C3-O31
39	c	527	LMK	O1-C7-C8-C9
39	c	527	LMK	C7-C8-C9-O8
45	I	102	4RF	C19-C20-C39-O40
45	k	101	4RF	O18-C19-C20-C39
31	b	621	SQD	C12-C13-C14-C15
38	C	525	LHG	C9-C10-C11-C12
38	C	525	LHG	C35-C36-C37-C38
38	G	624	LHG	C33-C34-C35-C36
38	G	624	LHG	C35-C36-C37-C38
38	L	101	LHG	C19-C20-C21-C22
38	d	410	LHG	C24-C25-C26-C27
51	Y	626	PTY	C35-C36-C37-C38
28	C	504	CLA	C8-C10-C11-C12
45	I	102	4RF	C25-C26-C27-C28
38	D	409	LHG	C13-C14-C15-C16
28	b	602	CLA	O1A-CGA-O2A-C1
28	b	615	CLA	C8-C10-C11-C12
37	b	625	DGA	CCA-CDA-CEA-CFA
32	A	413	LMG	C34-C35-C36-C37
35	c	518	DGD	C9B-CAB-CBB-CCB
45	k	101	4RF	C32-C33-C34-C35
39	C	527	LMK	C7-C8-O7-C10
39	C	527	LMK	C9-C8-O7-C10
28	B	617	CLA	O1A-CGA-O2A-C1
38	G	624	LHG	C26-C27-C28-C29
45	k	101	4RF	C46-C47-C48-C49
32	d	411	LMG	C30-C31-C32-C33
33	Y	625	SPH	C11-C12-C13-C14
37	C	524	DGA	CBB-CAB-CB9-CB8
38	c	525	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
38	N	624	LHG	O6-C4-C5-O7
38	d	409	LHG	O6-C4-C5-O7
32	a	413	LMG	C29-C28-O8-C9
28	b	612	CLA	C16-C17-C18-C19
28	N	610	CLA	C5-C6-C7-C8
32	C	521	LMG	O7-C10-C11-C12
38	D	410	LHG	O2-C2-C3-O3
32	A	413	LMG	C40-C41-C42-C43
38	D	408	LHG	C28-C29-C30-C31
38	S	624	LHG	C26-C27-C28-C29
38	d	409	LHG	C35-C36-C37-C38
28	Y	613	CLA	C13-C15-C16-C17
38	N	624	LHG	C31-C32-C33-C34
45	K	101	4RF	C12-C13-C14-C15
35	c	518	DGD	O6D-C5D-C6D-O5D
31	B	626	SQD	O6-C44-C45-O47
35	B	623	DGD	O1G-C1G-C2G-O2G
38	L	101	LHG	O7-C5-C6-O8
45	i	101	4RF	O18-C19-C20-O21
37	b	625	DGA	CAA-CBA-CCA-CDA
38	d	409	LHG	C30-C31-C32-C33
46	S	608	CHL	C11-C12-C13-C15
31	a	412	SQD	C15-C16-C17-C18
45	K	101	4RF	C29-C30-C31-C32
45	k	101	4RF	C49-C50-C51-C52
32	a	413	LMG	O6-C1-O1-C7
38	d	409	LHG	C1-C2-C3-O3
31	B	621	SQD	C14-C15-C16-C17
31	b	626	SQD	C19-C20-C21-C22
33	a	414	SPH	C10-C11-C12-C13
35	c	519	DGD	C2A-C3A-C4A-C5A
37	b	625	DGA	CB6-CB7-CB8-CB9
38	D	409	LHG	C35-C36-C37-C38
38	N	624	LHG	C35-C36-C37-C38
41	d	405	PL9	C40-C39-C41-C42
28	N	602	CLA	C2-C1-O2A-CGA
28	G	610	CLA	C2-C1-O2A-CGA
28	Y	602	CLA	C2-C1-O2A-CGA
28	Y	610	CLA	C2-C1-O2A-CGA
28	c	511	CLA	C15-C16-C17-C18
28	B	602	CLA	C14-C13-C15-C16
28	B	609	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	B	616	CLA	C11-C12-C13-C14
28	S	609	CLA	C6-C7-C8-C9
28	Y	602	CLA	C6-C7-C8-C9
28	Y	602	CLA	C11-C10-C8-C9
28	b	616	CLA	C11-C12-C13-C14
28	c	505	CLA	C11-C10-C8-C9
46	N	601	CHL	C14-C13-C15-C16
46	G	601	CHL	C6-C7-C8-C9
35	C	518	DGD	C2B-C3B-C4B-C5B
36	S	626	3PH	C2C-C2D-C2E-C2F
36	T	101	3PH	C2C-C2D-C2E-C2F
45	k	101	4RF	C35-C36-C37-C38
50	S	625	LPX	C13-C14-C15-C16
29	A	408	PHO	C1A-C2A-CAA-CBA
38	D	409	LHG	C2-C3-O3-P
38	l	101	LHG	C2-C3-O3-P
38	D	408	LHG	C11-C10-C9-C8
45	i	101	4RF	C51-C52-C53-C54
28	C	501	CLA	C2A-CAA-CBA-CGA
28	S	611	CLA	C2A-CAA-CBA-CGA
28	b	617	CLA	C2A-CAA-CBA-CGA
30	C	515	BCR	C23-C24-C25-C26
30	C	515	BCR	C23-C24-C25-C30
30	c	514	BCR	C23-C24-C25-C26
30	c	514	BCR	C23-C24-C25-C30
47	G	621	LUT	C1-C6-C7-C8
28	C	508	CLA	C10-C11-C12-C13
28	C	509	CLA	C15-C16-C17-C18
28	S	602	CLA	C8-C10-C11-C12
28	b	605	CLA	C5-C6-C7-C8
28	c	513	CLA	C8-C10-C11-C12
32	h	102	LMG	C15-C16-C17-C18
28	b	602	CLA	CAA-CBA-CGA-O2A
41	D	405	PL9	C47-C48-C49-C50
36	t	101	3PH	C38-C39-C3A-C3B
38	S	624	LHG	C14-C15-C16-C17
38	c	525	LHG	C34-C35-C36-C37
45	I	102	4RF	C52-C53-C54-C55
45	K	101	4RF	C03-C04-C05-C06
30	b	618	BCR	C17-C18-C19-C20
47	Y	620	LUT	C31-C32-C33-C34
49	Y	623	NEX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	A	405	CLA	C10-C11-C12-C13
28	B	611	CLA	C13-C15-C16-C17
51	Y	626	PTY	C11-C8-O7-C6
37	B	625	DGA	CBB-CAB-CB9-CB8
32	w	201	LMG	C37-C38-C39-C40
28	A	406	CLA	C3-C5-C6-C7
28	a	405	CLA	C13-C15-C16-C17
31	A	412	SQD	C10-C11-C12-C13
38	G	624	LHG	C24-C25-C26-C27
28	c	513	CLA	O1A-CGA-O2A-C1
39	c	527	LMK	O7-C10-C11-C12
38	L	101	LHG	O6-C4-C5-C6
38	c	525	LHG	O6-C4-C5-C6
38	l	101	LHG	O6-C4-C5-C6
36	b	624	3PH	C22-C23-C24-C25
28	B	602	CLA	C12-C13-C15-C16
28	B	604	CLA	C11-C12-C13-C15
28	B	604	CLA	C12-C13-C15-C16
28	B	607	CLA	C11-C10-C8-C7
28	B	609	CLA	C11-C10-C8-C7
28	B	616	CLA	C6-C7-C8-C10
28	B	617	CLA	C6-C7-C8-C10
28	C	501	CLA	C12-C13-C15-C16
28	C	505	CLA	C12-C13-C15-C16
28	C	507	CLA	C12-C13-C15-C16
28	C	509	CLA	C6-C7-C8-C10
28	C	509	CLA	C12-C13-C15-C16
28	C	510	CLA	C12-C13-C15-C16
28	C	512	CLA	C11-C10-C8-C7
28	C	513	CLA	C6-C7-C8-C10
28	N	603	CLA	C12-C13-C15-C16
28	G	602	CLA	C6-C7-C8-C10
28	G	602	CLA	C12-C13-C15-C16
28	G	610	CLA	C11-C10-C8-C7
28	S	609	CLA	C6-C7-C8-C10
28	S	610	CLA	C11-C10-C8-C7
28	Y	602	CLA	C6-C7-C8-C10
28	Y	612	CLA	C11-C10-C8-C7
28	Y	613	CLA	C11-C12-C13-C15
28	Y	613	CLA	C12-C13-C15-C16
28	b	602	CLA	C12-C13-C15-C16
28	b	604	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
28	b	613	CLA	C11-C10-C8-C7
28	c	501	CLA	C11-C10-C8-C7
28	c	504	CLA	C6-C7-C8-C10
28	c	504	CLA	C11-C10-C8-C7
28	c	513	CLA	C11-C12-C13-C15
28	d	402	CLA	C11-C10-C8-C7
28	d	403	CLA	C11-C12-C13-C15
28	d	403	CLA	C12-C13-C15-C16
46	N	601	CHL	C12-C13-C15-C16
46	N	606	CHL	C11-C10-C8-C7
46	N	607	CHL	C11-C12-C13-C15
46	G	601	CHL	C6-C7-C8-C10
46	Y	606	CHL	C6-C7-C8-C10
31	m	101	SQD	C26-C27-C28-C29
30	A	411	BCR	C9-C10-C11-C12
30	b	618	BCR	C13-C14-C15-C16
30	b	619	BCR	C19-C20-C21-C22
30	c	515	BCR	C19-C20-C21-C22
30	d	404	BCR	C19-C20-C21-C22
28	A	410	CLA	C11-C12-C13-C14
28	B	617	CLA	C16-C17-C18-C19
38	d	410	LHG	C24-C23-O8-C6
28	a	405	CLA	C8-C10-C11-C12
37	C	524	DGA	CA4-CA5-CA6-CA7
38	D	408	LHG	C13-C14-C15-C16
38	S	624	LHG	C34-C35-C36-C37
29	a	409	PHO	C3-C5-C6-C7
28	C	513	CLA	CBA-CGA-O2A-C1
28	D	402	CLA	CAA-CBA-CGA-O2A
37	B	625	DGA	CA9-CAA-CBA-CCA
37	B	625	DGA	CFA-CGA-CHA-CIA
45	k	101	4RF	C11-C12-C13-C14
35	C	518	DGD	O6D-C5D-C6D-O5D
28	B	602	CLA	CAD-CBD-CGD-O2D
28	B	608	CLA	CAD-CBD-CGD-O2D
28	C	502	CLA	CAD-CBD-CGD-O2D
28	G	602	CLA	CAD-CBD-CGD-O2D
28	G	603	CLA	CAD-CBD-CGD-O2D
28	Y	604	CLA	CAD-CBD-CGD-O2D
28	c	501	CLA	CAD-CBD-CGD-O2D
28	c	512	CLA	CAD-CBD-CGD-O2D
29	A	408	PHO	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	m	101	SQD	C46-C45-O47-C7
36	S	626	3PH	C1-C2-O21-C21
46	N	607	CHL	CAD-CBD-CGD-O2D
51	Y	626	PTY	O10-C8-O7-C6
28	c	505	CLA	C4-C3-C5-C6
31	b	626	SQD	O6-C44-C45-C46
36	T	101	3PH	C1-C2-C3-O31
38	C	525	LHG	C4-C5-C6-O8
38	N	624	LHG	C4-C5-C6-O8
38	G	624	LHG	C4-C5-C6-O8
38	d	408	LHG	C2-C3-O3-P
45	I	102	4RF	O18-C19-C20-C39
36	b	624	3PH	O11-C1-C2-O21
38	D	410	LHG	O6-C4-C5-O7
38	c	525	LHG	O6-C4-C5-O7
28	N	613	CLA	C10-C11-C12-C13
28	b	603	CLA	C10-C11-C12-C13
28	B	612	CLA	C10-C11-C12-C13
28	a	406	CLA	C5-C6-C7-C8
31	b	626	SQD	C10-C11-C12-C13
28	B	605	CLA	CHA-CBD-CGD-O1D
28	B	605	CLA	CHA-CBD-CGD-O2D
28	B	607	CLA	CHA-CBD-CGD-O1D
28	B	607	CLA	CHA-CBD-CGD-O2D
28	B	609	CLA	CHA-CBD-CGD-O1D
28	B	609	CLA	CHA-CBD-CGD-O2D
28	B	613	CLA	CHA-CBD-CGD-O1D
28	B	613	CLA	CHA-CBD-CGD-O2D
28	C	504	CLA	CHA-CBD-CGD-O1D
28	C	504	CLA	CHA-CBD-CGD-O2D
28	C	506	CLA	CHA-CBD-CGD-O1D
28	C	506	CLA	CHA-CBD-CGD-O2D
28	C	507	CLA	CHA-CBD-CGD-O1D
28	C	507	CLA	CHA-CBD-CGD-O2D
28	N	604	CLA	CHA-CBD-CGD-O1D
28	N	604	CLA	CHA-CBD-CGD-O2D
28	G	604	CLA	CHA-CBD-CGD-O1D
28	G	604	CLA	CHA-CBD-CGD-O2D
28	G	612	CLA	CHA-CBD-CGD-O1D
28	G	612	CLA	CHA-CBD-CGD-O2D
28	Y	602	CLA	CHA-CBD-CGD-O1D
28	Y	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	Y	612	CLA	CHA-CBD-CGD-O1D
28	Y	612	CLA	CHA-CBD-CGD-O2D
28	b	613	CLA	CHA-CBD-CGD-O1D
28	b	613	CLA	CHA-CBD-CGD-O2D
28	b	617	CLA	CHA-CBD-CGD-O1D
28	b	617	CLA	CHA-CBD-CGD-O2D
28	c	503	CLA	CHA-CBD-CGD-O1D
28	c	503	CLA	CHA-CBD-CGD-O2D
28	c	504	CLA	CHA-CBD-CGD-O1D
28	c	504	CLA	CHA-CBD-CGD-O2D
28	c	505	CLA	CHA-CBD-CGD-O1D
28	c	505	CLA	CHA-CBD-CGD-O2D
28	c	506	CLA	CHA-CBD-CGD-O1D
46	N	601	CHL	CHA-CBD-CGD-O1D
46	N	601	CHL	CHA-CBD-CGD-O2D
46	N	609	CHL	CHA-CBD-CGD-O1D
46	N	609	CHL	CHA-CBD-CGD-O2D
45	K	101	4RF	O17-C16-O18-C19
30	c	516	BCR	C11-C10-C9-C8
32	a	413	LMG	C11-C12-C13-C14
37	C	524	DGA	CCB-CDB-CEB-CFB
31	C	526	SQD	O6-C44-C45-O47
31	b	626	SQD	O6-C44-C45-O47
32	H	102	LMG	O7-C8-C9-O8
32	a	413	LMG	O7-C8-C9-O8
32	c	521	LMG	O7-C8-C9-O8
35	b	623	DGD	O1G-C1G-C2G-O2G
36	t	101	3PH	O21-C2-C3-O31
38	C	525	LHG	O7-C5-C6-O8
38	S	624	LHG	O7-C5-C6-O8
31	B	621	SQD	C12-C13-C14-C15
38	l	101	LHG	C12-C13-C14-C15
38	Y	624	LHG	C26-C27-C28-C29
31	M	101	SQD	C11-C10-C9-C8
37	B	625	DGA	CEA-CFA-CGA-CHA
38	L	101	LHG	C30-C31-C32-C33
46	Y	609	CHL	C4-C3-C5-C6
32	a	413	LMG	O10-C28-O8-C9
41	D	405	PL9	C4-C3-C7-C8
31	m	101	SQD	C10-C11-C12-C13
38	C	525	LHG	C24-C25-C26-C27
32	w	201	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	C	512	CLA	C11-C10-C8-C9
28	D	403	CLA	C11-C12-C13-C14
28	N	602	CLA	C6-C7-C8-C9
28	N	610	CLA	C11-C12-C13-C14
28	S	610	CLA	C11-C10-C8-C9
28	Y	613	CLA	C11-C12-C13-C14
28	Y	613	CLA	C14-C13-C15-C16
28	c	503	CLA	C14-C13-C15-C16
46	N	606	CHL	C11-C12-C13-C14
35	C	518	DGD	C4A-C5A-C6A-C7A
36	t	101	3PH	C35-C36-C37-C38
38	d	408	LHG	C34-C35-C36-C37
28	C	513	CLA	O1A-CGA-O2A-C1
31	a	412	SQD	C4-C5-C6-S
31	b	621	SQD	C4-C5-C6-S
31	c	526	SQD	C4-C5-C6-S
31	m	101	SQD	C4-C5-C6-S
31	B	626	SQD	C12-C13-C14-C15
38	G	624	LHG	C31-C32-C33-C34
28	B	607	CLA	C2A-CAA-CBA-CGA
28	G	610	CLA	C2A-CAA-CBA-CGA
46	Y	605	CHL	C2A-CAA-CBA-CGA
31	M	101	SQD	O47-C7-C8-C9
31	B	626	SQD	C32-C33-C34-C35
30	c	515	BCR	C37-C22-C23-C24
30	C	516	BCR	C21-C22-C23-C24
30	c	517	BCR	C21-C22-C23-C24
36	B	624	3PH	C35-C36-C37-C38
28	A	410	CLA	C1A-C2A-CAA-CBA
28	C	512	CLA	C1A-C2A-CAA-CBA
28	D	403	CLA	C1A-C2A-CAA-CBA
28	G	611	CLA	C1A-C2A-CAA-CBA
28	b	602	CLA	C1A-C2A-CAA-CBA
28	c	508	CLA	C1A-C2A-CAA-CBA
28	d	403	CLA	C1A-C2A-CAA-CBA
28	G	603	CLA	C16-C17-C18-C19
36	T	101	3PH	C38-C39-C3A-C3B
28	B	611	CLA	C2-C1-O2A-CGA
28	N	603	CLA	C2-C1-O2A-CGA
28	N	614	CLA	C2-C1-O2A-CGA
28	b	603	CLA	C2-C1-O2A-CGA
29	A	408	PHO	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	a	408	PHO	CBA-CGA-O2A-C1
38	C	525	LHG	C24-C23-O8-C6
45	i	101	4RF	C32-C33-C34-C35
43	H	101	RRX	C19-C20-C21-C22
38	S	624	LHG	C3-O3-P-O6
31	B	621	SQD	C25-C26-C27-C28
37	c	524	DGA	CCA-CDA-CEA-CFA
45	i	101	4RF	C29-C30-C31-C32
45	i	101	4RF	C47-C48-C49-C50
36	b	624	3PH	C2-C1-O11-P
38	S	624	LHG	C2-C3-O3-P
28	S	602	CLA	C2-C3-C5-C6
31	b	621	SQD	C25-C26-C27-C28
45	k	101	4RF	C25-C26-C27-C28
38	C	525	LHG	C3-O3-P-O4
38	D	410	LHG	C4-O6-P-O4
38	d	408	LHG	C3-O3-P-O5
38	d	410	LHG	C3-O3-P-O4
50	S	625	LPX	C3-O1-P1-O4
51	Y	627	PTY	C5-O14-P1-O13
28	B	608	CLA	C16-C17-C18-C20
28	Y	604	CLA	C16-C17-C18-C19
28	b	612	CLA	C16-C17-C18-C20
31	C	526	SQD	O5-C1-O6-C44
28	c	510	CLA	C13-C15-C16-C17
28	C	505	CLA	C15-C16-C17-C18
28	Y	610	CLA	C15-C16-C17-C18
28	B	611	CLA	C2A-CAA-CBA-CGA
28	C	505	CLA	C3-C5-C6-C7
46	N	607	CHL	C3-C5-C6-C7
46	S	608	CHL	C3-C5-C6-C7
36	S	626	3PH	C2F-C2G-C2H-C2I
28	B	605	CLA	CAD-CBD-CGD-O1D
28	B	613	CLA	CAD-CBD-CGD-O1D
28	C	504	CLA	CAD-CBD-CGD-O1D
28	C	506	CLA	CAD-CBD-CGD-O1D
28	G	604	CLA	CAD-CBD-CGD-O1D
28	S	611	CLA	CAD-CBD-CGD-O1D
28	c	503	CLA	CAD-CBD-CGD-O1D
28	c	504	CLA	CAD-CBD-CGD-O1D
28	c	506	CLA	CAD-CBD-CGD-O1D
28	c	510	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	B	626	SQD	O5-C5-C6-S
39	C	527	LMK	C29-C28-O8-C9
46	N	601	CHL	CAD-CBD-CGD-O1D
46	N	609	CHL	CAD-CBD-CGD-O1D
35	B	623	DGD	C1B-C2B-C3B-C4B
32	b	622	LMG	C18-C19-C20-C21
36	b	624	3PH	C32-C33-C34-C35
32	a	413	LMG	C30-C31-C32-C33
38	Y	624	LHG	C35-C36-C37-C38
28	D	402	CLA	C3-C5-C6-C7
32	C	523	LMG	C11-C12-C13-C14
38	S	624	LHG	C33-C34-C35-C36
38	c	525	LHG	C15-C16-C17-C18
45	i	101	4RF	C49-C50-C51-C52
28	B	608	CLA	C11-C12-C13-C15
28	B	613	CLA	C11-C10-C8-C7
28	B	616	CLA	C11-C12-C13-C15
28	C	506	CLA	C11-C10-C8-C7
28	C	507	CLA	C11-C12-C13-C15
28	C	509	CLA	C11-C10-C8-C7
28	C	512	CLA	C11-C12-C13-C15
28	C	513	CLA	C11-C10-C8-C7
28	D	403	CLA	C11-C12-C13-C15
28	N	602	CLA	C6-C7-C8-C10
28	N	610	CLA	C11-C12-C13-C15
28	N	610	CLA	C12-C13-C15-C16
28	S	610	CLA	C11-C12-C13-C15
28	S	611	CLA	C11-C12-C13-C15
28	b	603	CLA	C6-C7-C8-C10
28	b	604	CLA	C12-C13-C15-C16
28	b	606	CLA	C6-C7-C8-C10
28	b	608	CLA	C11-C10-C8-C7
28	b	609	CLA	C11-C12-C13-C15
28	c	503	CLA	C12-C13-C15-C16
28	c	505	CLA	C6-C7-C8-C10
38	C	525	LHG	O6-C4-C5-O7
38	D	408	LHG	O6-C4-C5-O7
38	L	101	LHG	O6-C4-C5-O7
38	d	408	LHG	O6-C4-C5-O7
38	l	101	LHG	O6-C4-C5-O7
41	D	405	PL9	C13-C14-C16-C17
46	N	606	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
46	G	607	CHL	C6-C7-C8-C10
46	Y	609	CHL	C11-C12-C13-C15
51	Y	627	PTY	O14-C5-C6-O7
38	D	409	LHG	C27-C28-C29-C30
29	a	408	PHO	O1A-CGA-O2A-C1
31	a	412	SQD	C24-C25-C26-C27
30	C	514	BCR	C19-C20-C21-C22
35	c	518	DGD	C4D-C5D-C6D-O5D
32	H	102	LMG	O7-C10-C11-C12
38	L	101	LHG	C14-C15-C16-C17
38	Y	624	LHG	C32-C33-C34-C35
28	N	604	CLA	C2A-CAA-CBA-CGA
28	b	608	CLA	C16-C17-C18-C20
36	T	101	3PH	C3D-C3E-C3F-C3G
37	C	524	DGA	CA2-CA3-CA4-CA5
35	C	518	DGD	C4D-C5D-C6D-O5D
46	S	608	CHL	CAA-CBA-CGA-O2A
31	B	626	SQD	O6-C44-C45-C46
31	C	526	SQD	O6-C44-C45-C46
33	A	414	SPH	C1-C2-C3-C4
36	b	624	3PH	C1-C2-C3-O31
37	j	101	DGA	CB5-CB6-CB7-CB8
38	D	409	LHG	C16-C17-C18-C19
38	D	410	LHG	C4-C5-C6-O8
45	K	101	4RF	C19-C20-C39-O40
31	C	526	SQD	O47-C45-C46-O48
31	M	101	SQD	O47-C45-C46-O48
31	a	412	SQD	O6-C44-C45-O47
32	b	622	LMG	O7-C8-C9-O8
32	w	201	LMG	O1-C7-C8-O7
31	A	412	SQD	C14-C15-C16-C17
32	c	523	LMG	C33-C34-C35-C36
29	A	408	PHO	O1A-CGA-O2A-C1
38	D	410	LHG	C11-C10-C9-C8
31	A	412	SQD	C45-C44-O6-C1
32	w	201	LMG	C8-C7-O1-C1
35	C	519	DGD	C5D-C6D-O5D-C1E
35	c	519	DGD	C5D-C6D-O5D-C1E
28	B	611	CLA	C8-C10-C11-C12
28	B	616	CLA	O1A-CGA-O2A-C1
28	S	610	CLA	C4-C3-C5-C6
28	B	616	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	B	626	SQD	C24-C23-O48-C46
45	K	101	4RF	C50-C51-C52-C53
28	N	602	CLA	C10-C11-C12-C13
28	A	406	CLA	C11-C10-C8-C9
28	C	502	CLA	C11-C10-C8-C9
28	C	507	CLA	C14-C13-C15-C16
28	C	510	CLA	C14-C13-C15-C16
28	G	602	CLA	C6-C7-C8-C9
28	G	602	CLA	C14-C13-C15-C16
28	G	610	CLA	C11-C10-C8-C9
28	b	604	CLA	C6-C7-C8-C9
28	b	609	CLA	C11-C12-C13-C14
28	b	611	CLA	C11-C12-C13-C14
28	c	501	CLA	C11-C10-C8-C9
31	b	626	SQD	C30-C31-C32-C33
32	H	102	LMG	C12-C13-C14-C15
28	d	402	CLA	CAA-CBA-CGA-O2A
32	C	523	LMG	C14-C15-C16-C17
38	S	624	LHG	C29-C30-C31-C32
38	d	409	LHG	C33-C34-C35-C36
38	l	101	LHG	C35-C36-C37-C38
28	c	507	CLA	C15-C16-C17-C18
38	d	410	LHG	O10-C23-O8-C6
37	c	524	DGA	CFA-CGA-CHA-CIA
38	N	624	LHG	C30-C31-C32-C33
31	C	526	SQD	C29-C30-C31-C32
35	c	520	DGD	C4A-C5A-C6A-C7A
38	d	408	LHG	C35-C36-C37-C38
38	l	101	LHG	C29-C30-C31-C32
45	k	101	4RF	C33-C34-C35-C36
30	a	411	BCR	C11-C12-C13-C14
33	A	414	SPH	C10-C11-C12-C13
35	c	520	DGD	O6D-C5D-C6D-O5D
36	B	624	3PH	C39-C3A-C3B-C3C
38	D	409	LHG	C33-C34-C35-C36
28	N	611	CLA	C1-C2-C3-C4
28	G	604	CLA	C1-C2-C3-C4
28	G	614	CLA	C1-C2-C3-C4
33	a	414	SPH	C2-C3-C4-C5
46	N	608	CHL	C1-C2-C3-C4
46	G	606	CHL	C1-C2-C3-C4
28	B	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	B	602	CLA	C3-C5-C6-C7
28	a	405	CLA	CAA-CBA-CGA-O2A
31	M	101	SQD	C46-C45-O47-C7
31	b	621	SQD	C46-C45-O47-C7
32	B	622	LMG	C9-C8-O7-C10
32	b	622	LMG	C9-C8-O7-C10
38	l	101	LHG	C6-C5-O7-C7
32	B	622	LMG	C11-C12-C13-C14
28	A	410	CLA	C2-C1-O2A-CGA
28	B	604	CLA	C2-C1-O2A-CGA
28	C	513	CLA	C2-C1-O2A-CGA
28	D	402	CLA	C2-C1-O2A-CGA
28	N	610	CLA	C2-C1-O2A-CGA
28	b	612	CLA	C2-C1-O2A-CGA
46	N	601	CHL	C2-C1-O2A-CGA
46	Y	609	CHL	C2-C1-O2A-CGA
32	C	521	LMG	C29-C30-C31-C32
45	k	101	4RF	C44-C45-C46-C47
28	A	405	CLA	CAA-CBA-CGA-O2A
28	C	511	CLA	C13-C15-C16-C17
31	B	626	SQD	O10-C23-O48-C46
38	G	624	LHG	C16-C17-C18-C19
38	D	410	LHG	C30-C31-C32-C33
37	C	524	DGA	CB3-CB4-CB5-CB6
50	S	625	LPX	C15-C16-C17-C18
47	G	620	LUT	C29-C30-C31-C32
38	C	525	LHG	O10-C23-O8-C6
36	B	624	3PH	O11-C1-C2-O21
38	G	624	LHG	O6-C4-C5-O7
38	N	624	LHG	C9-C10-C11-C12
38	d	410	LHG	C26-C27-C28-C29
28	C	510	CLA	C4-C3-C5-C6
30	C	517	BCR	C23-C24-C25-C26
46	G	601	CHL	C3-C5-C6-C7
47	G	621	LUT	C5-C6-C7-C8
28	c	505	CLA	C2-C3-C5-C6
46	Y	609	CHL	C2-C3-C5-C6
45	i	101	4RF	C26-C27-C28-C29
35	c	519	DGD	C3B-C4B-C5B-C6B
28	B	602	CLA	C16-C17-C18-C20
36	S	626	3PH	C22-C21-O21-C2
32	c	523	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
32	h	102	LMG	O6-C1-O1-C7
35	C	518	DGD	O6E-C1E-O5D-C6D
35	b	623	DGD	O6E-C1E-O5D-C6D
51	Y	626	PTY	C37-C38-C39-C40
35	b	623	DGD	C2E-C1E-O5D-C6D
49	N	623	NEX	C28-C29-C30-C31
35	c	518	DGD	C2B-C3B-C4B-C5B
38	D	410	LHG	C34-C35-C36-C37
38	l	101	LHG	O7-C5-C6-O8
39	C	527	LMK	O1-C7-C8-O7
38	D	408	LHG	C3-O3-P-O6
38	D	409	LHG	C3-O3-P-O6
38	L	101	LHG	C4-O6-P-O3
38	N	624	LHG	C3-O3-P-O6
38	G	624	LHG	C3-O3-P-O6
38	Y	624	LHG	C3-O3-P-O6
38	d	409	LHG	C3-O3-P-O6
38	d	409	LHG	C4-O6-P-O3
38	l	101	LHG	C4-O6-P-O3
50	S	625	LPX	C3-O1-P1-O2
51	Y	626	PTY	C3-O11-P1-O14
51	Y	626	PTY	C5-O14-P1-O11
51	Y	627	PTY	C3-O11-P1-O14
35	c	518	DGD	C4A-C5A-C6A-C7A
37	C	524	DGA	CB5-CB6-CB7-CB8
38	l	101	LHG	C17-C18-C19-C20
45	K	101	4RF	C07-C08-C09-C10
29	A	409	PHO	CHA-CBD-CGD-O1D
29	A	409	PHO	CHA-CBD-CGD-O2D
29	a	409	PHO	CHA-CBD-CGD-O1D
29	a	409	PHO	CHA-CBD-CGD-O2D
32	D	411	LMG	C28-C29-C30-C31
28	B	605	CLA	CBA-CGA-O2A-C1
31	B	621	SQD	C44-C45-C46-O48
32	B	622	LMG	C7-C8-C9-O8
32	H	102	LMG	C7-C8-C9-O8
35	c	518	DGD	O1G-C1G-C2G-C3G
51	Y	627	PTY	O4-C1-C6-C5
37	B	625	DGA	CA2-CA3-CA4-CA5
45	i	101	4RF	C01-C02-C03-C04
28	B	617	CLA	C5-C6-C7-C8
28	B	609	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
28	N	603	CLA	C11-C10-C8-C7
46	N	607	CHL	C12-C13-C15-C16
46	G	607	CHL	C11-C12-C13-C15
46	Y	606	CHL	C12-C13-C15-C16
46	Y	607	CHL	C6-C7-C8-C10
28	B	608	CLA	C11-C12-C13-C14
28	B	613	CLA	C11-C10-C8-C9
28	B	616	CLA	C6-C7-C8-C9
28	C	512	CLA	C11-C12-C13-C14
28	S	602	CLA	C6-C7-C8-C9
28	Y	611	CLA	C6-C7-C8-C9
28	b	613	CLA	C11-C10-C8-C9
28	c	505	CLA	C6-C7-C8-C9
28	c	511	CLA	C11-C10-C8-C9
28	d	402	CLA	C11-C10-C8-C9
46	G	607	CHL	C6-C7-C8-C9
28	B	608	CLA	C16-C17-C18-C19
38	N	624	LHG	C34-C35-C36-C37
36	b	624	3PH	C38-C39-C3A-C3B
28	C	504	CLA	C2A-CAA-CBA-CGA
28	b	613	CLA	C3-C5-C6-C7
37	b	625	DGA	CA3-CA4-CA5-CA6
37	B	625	DGA	CA6-CA7-CA8-CA9
38	S	624	LHG	C5-C4-O6-P
28	Y	612	CLA	C15-C16-C17-C18
28	S	605	CLA	C2C-C3C-CAC-CBC
32	C	521	LMG	C13-C14-C15-C16
28	Y	604	CLA	C4-C3-C5-C6
33	Y	625	SPH	C10-C11-C12-C13
28	d	403	CLA	C16-C17-C18-C20
29	A	408	PHO	C16-C17-C18-C19
28	b	605	CLA	CBA-CGA-O2A-C1
38	N	624	LHG	O10-C23-C24-C25
32	b	622	LMG	O6-C5-C6-O5
28	S	605	CLA	C4C-C3C-CAC-CBC
46	S	601	CHL	CAA-CBA-CGA-O2A
36	B	624	3PH	C2C-C2D-C2E-C2F
45	I	102	4RF	C03-C04-C05-C06
32	D	411	LMG	C18-C19-C20-C21
30	C	516	BCR	C19-C20-C21-C22
47	Y	620	LUT	C29-C30-C31-C32
28	G	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	G	603	CLA	C3-C5-C6-C7
51	Y	627	PTY	N1-C2-C3-O11
32	W	201	LMG	C29-C30-C31-C32
45	I	102	4RF	C05-C06-C07-C08
45	I	102	4RF	C49-C50-C51-C52
30	B	619	BCR	C10-C11-C12-C13
32	c	523	LMG	C30-C31-C32-C33
28	N	602	CLA	C3-C5-C6-C7
32	C	523	LMG	C36-C37-C38-C39
28	S	603	CLA	C4-C3-C5-C6
28	b	609	CLA	C4-C3-C5-C6
46	Y	605	CHL	CAA-CBA-CGA-O1A
32	B	622	LMG	C19-C20-C21-C22
45	I	102	4RF	C43-C44-C45-C46
28	B	610	CLA	C2-C1-O2A-CGA
28	D	403	CLA	C2-C1-O2A-CGA
46	Y	606	CHL	C2-C1-O2A-CGA
32	c	523	LMG	C2-C1-O1-C7
35	C	518	DGD	C2E-C1E-O5D-C6D
45	k	101	4RF	O18-C19-C20-O21
45	I	102	4RF	C47-C48-C49-C50
28	b	605	CLA	CAA-CBA-CGA-O2A
38	L	101	LHG	C2-C3-O3-P
28	c	511	CLA	C3A-C2A-CAA-CBA
28	c	512	CLA	C3A-C2A-CAA-CBA
46	N	607	CHL	C3A-C2A-CAA-CBA
46	Y	601	CHL	C3A-C2A-CAA-CBA
31	m	101	SQD	O47-C7-C8-C9
38	G	624	LHG	O8-C23-C24-C25
30	A	411	BCR	C19-C20-C21-C22
28	C	501	CLA	C13-C15-C16-C17
36	B	624	3PH	C2F-C2G-C2H-C2I
36	S	626	3PH	C3C-C3D-C3E-C3F
28	b	604	CLA	C4-C3-C5-C6
28	c	509	CLA	C4-C3-C5-C6
31	C	526	SQD	C11-C10-C9-C8
38	D	408	LHG	C34-C35-C36-C37
28	S	610	CLA	C2-C3-C5-C6
32	c	521	LMG	O7-C10-C11-C12
28	B	606	CLA	C6-C7-C8-C9
28	B	614	CLA	C14-C13-C15-C16
28	C	503	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
28	C	507	CLA	C11-C12-C13-C14
28	N	610	CLA	C14-C13-C15-C16
28	S	610	CLA	C11-C12-C13-C14
28	Y	603	CLA	C6-C7-C8-C9
28	a	405	CLA	C14-C13-C15-C16
28	c	501	CLA	C11-C12-C13-C14
28	c	506	CLA	C6-C7-C8-C9
46	N	607	CHL	C14-C13-C15-C16
46	G	607	CHL	C11-C10-C8-C9
46	Y	609	CHL	C11-C10-C8-C9
28	Y	604	CLA	C16-C17-C18-C20
35	c	518	DGD	CAB-CBB-CCB-CDB
38	L	101	LHG	C29-C30-C31-C32
51	Y	626	PTY	C11-C12-C13-C14
38	c	525	LHG	C10-C11-C12-C13
37	C	524	DGA	OG1-CG1-CG2-CG3
38	d	409	LHG	C4-C5-C6-O8
49	N	623	NEX	C39-C29-C30-C31
49	S	623	NEX	C39-C29-C30-C31
41	d	405	PL9	C17-C18-C19-C21
28	N	611	CLA	C2A-CAA-CBA-CGA
28	C	511	CLA	C5-C6-C7-C8
38	l	101	LHG	C34-C35-C36-C37
28	b	608	CLA	C16-C17-C18-C19
31	B	626	SQD	C13-C14-C15-C16
38	d	410	LHG	C9-C10-C11-C12
45	i	101	4RF	C25-C26-C27-C28
35	C	519	DGD	C2A-C3A-C4A-C5A
28	b	609	CLA	C15-C16-C17-C18
31	b	626	SQD	C31-C32-C33-C34
38	D	410	LHG	C9-C10-C11-C12
31	c	526	SQD	C25-C26-C27-C28
35	B	623	DGD	C1G-C2G-O2G-C1B
35	b	623	DGD	C1G-C2G-O2G-C1B
38	L	101	LHG	C6-C5-O7-C7
28	Y	603	CLA	C4-C3-C5-C6
28	B	604	CLA	C1A-C2A-CAA-CBA
28	N	602	CLA	C1A-C2A-CAA-CBA
28	b	605	CLA	C1A-C2A-CAA-CBA
45	K	101	4RF	C43-C44-C45-C46
28	C	502	CLA	C6-C7-C8-C10
28	Y	612	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	Y	614	CLA	C11-C10-C8-C7
28	b	613	CLA	C6-C7-C8-C10
28	c	512	CLA	C6-C7-C8-C10
46	Y	605	CHL	CAA-CBA-CGA-O2A
37	c	524	DGA	CDA-CEA-CFA-CGA
32	h	102	LMG	O7-C10-C11-C12
31	a	412	SQD	C14-C15-C16-C17
38	N	624	LHG	C19-C20-C21-C22
28	C	509	CLA	C8-C10-C11-C12
28	C	503	CLA	C3-C5-C6-C7
28	c	503	CLA	C3-C5-C6-C7
28	N	613	CLA	C2A-CAA-CBA-CGA
28	B	606	CLA	C10-C11-C12-C13
28	B	606	CLA	C15-C16-C17-C18
36	S	626	3PH	C25-C26-C27-C28
45	i	101	4RF	C53-C54-C55-C56
51	Y	626	PTY	C24-C25-C26-C27
36	S	626	3PH	O11-C1-C2-O21
45	k	101	4RF	C09-C10-C11-C12
37	j	101	DGA	CA2-CA3-CA4-CA5
28	Y	614	CLA	C16-C17-C18-C19
28	b	615	CLA	C16-C17-C18-C20
46	S	601	CHL	CAA-CBA-CGA-O1A
41	d	405	PL9	C30-C29-C31-C32
31	B	626	SQD	C11-C10-C9-C8
35	c	518	DGD	C6B-C7B-C8B-C9B
28	c	508	CLA	C13-C15-C16-C17
28	C	510	CLA	C2-C3-C5-C6
28	Y	604	CLA	C2-C3-C5-C6
28	c	509	CLA	C2-C3-C5-C6
45	k	101	4RF	C05-C06-C07-C08
38	G	624	LHG	C29-C30-C31-C32
28	b	611	CLA	C8-C10-C11-C12
31	a	412	SQD	O49-C7-O47-C45
49	S	623	NEX	C28-C29-C30-C31
35	C	520	DGD	C5A-C6A-C7A-C8A
37	c	524	DGA	CB2-CB3-CB4-CB5
28	c	504	CLA	C2A-CAA-CBA-CGA
38	L	101	LHG	C35-C36-C37-C38
30	D	404	BCR	C19-C20-C21-C22
30	c	514	BCR	C13-C14-C15-C16
31	a	412	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
28	S	603	CLA	C16-C17-C18-C19
35	C	520	DGD	C4A-C5A-C6A-C7A
35	c	519	DGD	C2B-C3B-C4B-C5B
28	b	614	CLA	C13-C15-C16-C17
41	D	405	PL9	C39-C41-C42-C43
28	B	612	CLA	C4-C3-C5-C6
28	C	512	CLA	C4-C3-C5-C6
46	N	609	CHL	C4-C3-C5-C6
28	B	612	CLA	C2-C1-O2A-CGA
28	C	501	CLA	C2-C1-O2A-CGA
28	b	605	CLA	O1A-CGA-O2A-C1
37	j	101	DGA	CA5-CA6-CA7-CA8
28	C	508	CLA	C11-C12-C13-C14
32	A	413	LMG	O9-C10-C11-C12
38	D	409	LHG	C24-C25-C26-C27
31	A	412	SQD	C15-C16-C17-C18
32	d	411	LMG	C12-C13-C14-C15
28	B	606	CLA	C2A-CAA-CBA-CGA
28	B	613	CLA	C2A-CAA-CBA-CGA
28	c	510	CLA	C2A-CAA-CBA-CGA
46	S	601	CHL	C2A-CAA-CBA-CGA
38	N	624	LHG	C18-C19-C20-C21
30	c	515	BCR	C1-C6-C7-C8
30	c	517	BCR	C23-C24-C25-C30
47	G	620	LUT	C1-C6-C7-C8
47	S	620	LUT	C1-C6-C7-C8
47	Y	621	LUT	C1-C6-C7-C8
46	G	607	CHL	C5-C6-C7-C8
32	d	411	LMG	C18-C19-C20-C21
38	D	408	LHG	C32-C33-C34-C35
38	l	101	LHG	C33-C34-C35-C36
28	N	613	CLA	CAA-CBA-CGA-O1A
30	a	411	BCR	C19-C20-C21-C22
34	b	620	C7Z	C13-C14-C15-C35
47	S	620	LUT	C29-C30-C31-C32
31	m	101	SQD	C11-C12-C13-C14
35	C	518	DGD	C2A-C3A-C4A-C5A
36	t	101	3PH	C29-C2A-C2B-C2C
28	C	506	CLA	C4-C3-C5-C6
46	G	607	CHL	C4-C3-C5-C6
29	A	408	PHO	C16-C17-C18-C20
28	D	402	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	N	603	CLA	C15-C16-C17-C18
46	S	608	CHL	C10-C11-C12-C13
28	Y	603	CLA	C2-C3-C5-C6
46	N	606	CHL	C3-C5-C6-C7
28	N	602	CLA	C5-C6-C7-C8
31	c	526	SQD	C27-C28-C29-C30
36	B	624	3PH	C26-C27-C28-C29
36	t	101	3PH	C24-C25-C26-C27
32	h	102	LMG	C11-C12-C13-C14
28	S	610	CLA	C13-C15-C16-C17
36	B	624	3PH	C2D-C2E-C2F-C2G
36	S	626	3PH	C34-C35-C36-C37
35	C	520	DGD	O6D-C5D-C6D-O5D
28	C	501	CLA	O1A-CGA-O2A-C1
38	D	408	LHG	O6-C4-C5-C6
38	Y	624	LHG	O6-C4-C5-C6
28	C	505	CLA	C11-C10-C8-C7
41	d	405	PL9	C18-C19-C21-C22
29	A	408	PHO	CBD-CGD-O2D-CED
36	T	101	3PH	C3A-C3B-C3C-C3D
45	I	102	4RF	C27-C28-C29-C30
37	j	101	DGA	OG2-CG2-CG3-OXT
49	G	623	NEX	C33-C34-C35-C15
31	A	412	SQD	O47-C7-C8-C9
45	K	101	4RF	C01-C02-C03-C04
32	B	622	LMG	O7-C8-C9-O8
29	A	408	PHO	O1D-CGD-O2D-CED
46	N	608	CHL	O2A-C1-C2-C3
46	G	606	CHL	O2A-C1-C2-C3
36	t	101	3PH	O31-C31-C32-C33
28	C	512	CLA	C2A-CAA-CBA-CGA
28	B	602	CLA	C16-C17-C18-C19
37	J	101	DGA	CA5-CA6-CA7-CA8
45	I	102	4RF	C30-C31-C32-C33
36	B	624	3PH	C2A-C2B-C2C-C2D
37	B	625	DGA	OG2-CB1-CB2-CB3
32	C	521	LMG	O9-C10-C11-C12
31	M	101	SQD	C26-C27-C28-C29
28	S	611	CLA	C4-C3-C5-C6
28	a	405	CLA	C4-C3-C5-C6
46	N	607	CHL	C4-C3-C5-C6
46	G	601	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	B	615	CLA	C13-C15-C16-C17
46	N	609	CHL	C2-C3-C5-C6
32	c	523	LMG	O7-C10-C11-C12
28	B	612	CLA	C11-C12-C13-C14
28	C	506	CLA	C11-C10-C8-C9
28	C	509	CLA	C11-C10-C8-C9
28	G	613	CLA	C14-C13-C15-C16
28	S	611	CLA	C11-C12-C13-C14
28	a	405	CLA	C11-C12-C13-C14
28	b	603	CLA	C6-C7-C8-C9
28	b	609	CLA	C6-C7-C8-C9
28	b	610	CLA	C11-C12-C13-C14
28	b	612	CLA	C11-C10-C8-C9
28	c	507	CLA	C11-C12-C13-C14
28	c	510	CLA	C11-C12-C13-C14
28	d	403	CLA	C6-C7-C8-C9
29	a	409	PHO	C6-C7-C8-C9
46	G	609	CHL	C14-C13-C15-C16
46	Y	606	CHL	C11-C12-C13-C14
33	A	414	SPH	C2-C3-C4-C5
36	S	626	3PH	C3B-C3C-C3D-C3E
28	b	614	CLA	C3A-C2A-CAA-CBA
31	b	626	SQD	C15-C16-C17-C18
38	N	624	LHG	O2-C2-C3-O3
28	Y	613	CLA	CAA-CBA-CGA-O2A
28	C	510	CLA	CAD-CBD-CGD-O2D
28	C	512	CLA	CAD-CBD-CGD-O2D
28	N	602	CLA	CAD-CBD-CGD-O2D
28	N	603	CLA	CAD-CBD-CGD-O2D
28	N	612	CLA	CAD-CBD-CGD-O2D
28	S	612	CLA	CAD-CBD-CGD-O2D
28	Y	603	CLA	CAD-CBD-CGD-O2D
28	Y	614	CLA	CAD-CBD-CGD-O2D
28	b	606	CLA	CAD-CBD-CGD-O2D
28	b	608	CLA	CAD-CBD-CGD-O2D
38	L	101	LHG	C4-C5-O7-C7
46	S	606	CHL	CAD-CBD-CGD-O2D
46	Y	605	CHL	CAD-CBD-CGD-O2D
41	d	405	PL9	C12-C13-C14-C15
32	a	413	LMG	C29-C30-C31-C32
28	N	604	CLA	CAA-CBA-CGA-O2A
28	S	614	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	c	503	CLA	CAA-CBA-CGA-O2A
37	j	101	DGA	OG2-CB1-CB2-CB3
38	L	101	LHG	O9-C7-C8-C9
45	i	101	4RF	C24-C25-C26-C27
32	A	413	LMG	C33-C34-C35-C36
28	G	613	CLA	C4-C3-C5-C6
28	a	406	CLA	C4-C3-C5-C6
36	t	101	3PH	C2E-C2F-C2G-C2H
28	B	612	CLA	C2-C3-C5-C6
41	d	405	PL9	C38-C39-C41-C42
46	G	607	CHL	C2-C3-C5-C6
28	B	615	CLA	CAA-CBA-CGA-O2A
45	i	101	4RF	O40-C41-C43-C44
30	c	515	BCR	C11-C12-C13-C14
30	c	515	BCR	C21-C22-C23-C24
45	K	101	4RF	C48-C49-C50-C51
45	K	101	4RF	C51-C52-C53-C54
38	d	409	LHG	C2-C3-O3-P
39	c	527	LMK	C11-C10-O7-C8
51	Y	626	PTY	O4-C1-C6-C5
38	c	525	LHG	C14-C15-C16-C17
38	D	409	LHG	O6-C4-C5-O7
38	Y	624	LHG	O6-C4-C5-O7
32	C	523	LMG	O7-C10-C11-C12
36	S	626	3PH	O21-C21-C22-C23
46	G	605	CHL	CAA-CBA-CGA-O2A
28	d	403	CLA	C16-C17-C18-C19
30	a	411	BCR	C10-C11-C12-C13
28	S	610	CLA	C8-C10-C11-C12
29	a	408	PHO	O2A-C1-C2-C3
46	Y	607	CHL	O2A-C1-C2-C3
31	a	412	SQD	C35-C36-C37-C38
28	b	603	CLA	CAA-CBA-CGA-O2A
28	S	612	CLA	CAA-CBA-CGA-O2A
28	S	603	CLA	C16-C17-C18-C20
37	B	625	DGA	CA1-CA2-CA3-CA4
38	d	409	LHG	O2-C2-C3-O3
31	M	101	SQD	O49-C7-C8-C9
28	B	611	CLA	CHA-CBD-CGD-O1D
28	B	611	CLA	CHA-CBD-CGD-O2D
28	B	614	CLA	CHA-CBD-CGD-O1D
28	B	614	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	C	509	CLA	CHA-CBD-CGD-O1D
28	C	509	CLA	CHA-CBD-CGD-O2D
28	C	511	CLA	CHA-CBD-CGD-O1D
28	C	511	CLA	CHA-CBD-CGD-O2D
28	D	402	CLA	CHA-CBD-CGD-O1D
28	D	402	CLA	CHA-CBD-CGD-O2D
28	N	610	CLA	CHA-CBD-CGD-O1D
28	N	610	CLA	CHA-CBD-CGD-O2D
28	G	610	CLA	CHA-CBD-CGD-O1D
28	G	610	CLA	CHA-CBD-CGD-O2D
28	G	613	CLA	CHA-CBD-CGD-O2D
28	S	610	CLA	CHA-CBD-CGD-O2D
28	Y	608	CLA	CHA-CBD-CGD-O1D
28	Y	608	CLA	CHA-CBD-CGD-O2D
28	Y	610	CLA	CHA-CBD-CGD-O1D
28	Y	610	CLA	CHA-CBD-CGD-O2D
28	Y	613	CLA	CHA-CBD-CGD-O1D
28	Y	613	CLA	CHA-CBD-CGD-O2D
28	a	407	CLA	CHA-CBD-CGD-O1D
28	a	407	CLA	CHA-CBD-CGD-O2D
28	a	410	CLA	CHA-CBD-CGD-O1D
28	a	410	CLA	CHA-CBD-CGD-O2D
28	b	611	CLA	CHA-CBD-CGD-O1D
28	b	611	CLA	CHA-CBD-CGD-O2D
28	c	502	CLA	CHA-CBD-CGD-O1D
28	c	502	CLA	CHA-CBD-CGD-O2D
28	c	506	CLA	CHA-CBD-CGD-O2D
28	c	507	CLA	CHA-CBD-CGD-O1D
28	c	507	CLA	CHA-CBD-CGD-O2D
28	c	509	CLA	CHA-CBD-CGD-O1D
28	c	509	CLA	CHA-CBD-CGD-O2D
39	C	527	LMK	C2-C3-C4-O3
46	Y	609	CHL	CHA-CBD-CGD-O1D
46	Y	609	CHL	CHA-CBD-CGD-O2D
49	G	623	NEX	C13-C14-C15-C35
28	S	612	CLA	CAA-CBA-CGA-O1A
28	G	613	CLA	CAA-CBA-CGA-O2A
31	C	526	SQD	C32-C33-C34-C35
28	C	506	CLA	C2-C3-C5-C6
31	b	626	SQD	C25-C26-C27-C28
36	S	626	3PH	C32-C33-C34-C35
36	B	624	3PH	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
38	D	410	LHG	C10-C11-C12-C13
36	S	626	3PH	O11-C1-C2-C3
38	D	409	LHG	O6-C4-C5-C6
28	B	603	CLA	CAA-CBA-CGA-O2A
28	G	603	CLA	CAA-CBA-CGA-O2A
45	K	101	4RF	O21-C22-C24-C25
32	h	102	LMG	O7-C8-C9-O8
32	C	521	LMG	C28-C29-C30-C31
28	B	608	CLA	CAA-CBA-CGA-O2A
28	B	609	CLA	CAA-CBA-CGA-O2A
28	b	615	CLA	CAA-CBA-CGA-O2A
37	c	524	DGA	OG2-CB1-CB2-CB3
38	d	409	LHG	O7-C7-C8-C9
29	A	408	PHO	CHA-CBD-CGD-O1D
33	A	414	SPH	N2-C2-C3-O3
28	b	608	CLA	C5-C6-C7-C8
28	C	501	CLA	CBA-CGA-O2A-C1
31	B	626	SQD	C10-C11-C12-C13
31	C	526	SQD	C33-C34-C35-C36
28	A	405	CLA	C11-C12-C13-C15
28	B	617	CLA	C11-C12-C13-C15
28	C	508	CLA	C11-C12-C13-C15
28	Y	603	CLA	C11-C10-C8-C7
28	b	605	CLA	C12-C13-C15-C16
28	b	609	CLA	C2-C3-C5-C6
28	b	612	CLA	C2-C3-C5-C6
28	c	507	CLA	C11-C12-C13-C15
46	Y	607	CHL	C11-C12-C13-C15
31	b	626	SQD	C35-C36-C37-C38
33	Y	625	SPH	C4-C5-C6-C7
28	B	607	CLA	CAA-CBA-CGA-O2A
31	M	101	SQD	O48-C23-C24-C25
32	W	201	LMG	O7-C10-C11-C12
28	C	504	CLA	C11-C10-C8-C9
28	N	603	CLA	C11-C10-C8-C9
28	Y	602	CLA	C11-C12-C13-C14
28	Y	603	CLA	C11-C10-C8-C9
28	Y	614	CLA	C11-C10-C8-C9
28	b	605	CLA	C14-C13-C15-C16
28	b	609	CLA	C14-C13-C15-C16
28	c	512	CLA	C6-C7-C8-C9
28	c	512	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	C	501	CLA	C15-C16-C17-C18
31	B	621	SQD	C4-C5-C6-S
38	d	409	LHG	C15-C16-C17-C18
45	i	101	4RF	C31-C32-C33-C34
28	b	607	CLA	C13-C15-C16-C17
28	b	603	CLA	C2A-CAA-CBA-CGA
46	G	606	CHL	C2A-CAA-CBA-CGA
46	Y	606	CHL	C2A-CAA-CBA-CGA
28	B	615	CLA	CAA-CBA-CGA-O1A
28	S	610	CLA	CAA-CBA-CGA-O2A
37	B	625	DGA	CBB-CCB-CDB-CEB
38	l	101	LHG	C19-C20-C21-C22
28	G	614	CLA	CAA-CBA-CGA-O2A
32	C	523	LMG	C12-C13-C14-C15
28	b	602	CLA	CAA-CBA-CGA-O1A
47	N	620	LUT	C27-C28-C29-C30
28	b	612	CLA	C13-C15-C16-C17
38	C	525	LHG	C16-C17-C18-C19
28	B	606	CLA	C1A-C2A-CAA-CBA
28	Y	604	CLA	C1A-C2A-CAA-CBA
28	b	614	CLA	C1A-C2A-CAA-CBA
28	c	506	CLA	C1A-C2A-CAA-CBA
38	d	410	LHG	C1-C2-C3-O3
46	Y	601	CHL	C1A-C2A-CAA-CBA
32	A	413	LMG	C36-C37-C38-C39
28	N	604	CLA	CAA-CBA-CGA-O1A
28	Y	613	CLA	CAA-CBA-CGA-O1A
28	c	503	CLA	CAA-CBA-CGA-O1A
36	t	101	3PH	O32-C31-C32-C33
37	B	625	DGA	OB1-CB1-CB2-CB3
39	c	527	LMK	C12-C13-C14-C15
28	c	509	CLA	C8-C10-C11-C12
45	i	101	4RF	O42-C41-C43-C44
45	i	101	4RF	O18-C19-C20-C39
28	N	614	CLA	CAA-CBA-CGA-O2A
37	b	625	DGA	OG1-CA1-CA2-CA3
28	A	406	CLA	C2A-CAA-CBA-CGA
28	b	608	CLA	C2A-CAA-CBA-CGA
35	c	520	DGD	CCB-CDB-CEB-CFB
31	A	412	SQD	O49-C7-C8-C9
32	c	523	LMG	O9-C10-C11-C12
31	m	101	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
28	c	513	CLA	C10-C11-C12-C13
31	M	101	SQD	C10-C11-C12-C13
37	C	524	DGA	CA1-CA2-CA3-CA4
28	B	603	CLA	CAA-CBA-CGA-O1A
28	B	609	CLA	CAA-CBA-CGA-O1A
28	S	603	CLA	C2-C3-C5-C6
31	C	526	SQD	C2-C1-O6-C44
38	L	101	LHG	C4-O6-P-O5
38	N	624	LHG	C4-O6-P-O5
38	d	409	LHG	C4-O6-P-O5
38	l	101	LHG	C4-O6-P-O5
51	Y	626	PTY	C3-O11-P1-O13
32	c	521	LMG	C10-C11-C12-C13
31	m	101	SQD	C28-C29-C30-C31
28	B	607	CLA	CAA-CBA-CGA-O1A
28	G	613	CLA	CAA-CBA-CGA-O1A
31	M	101	SQD	O10-C23-C24-C25
37	c	524	DGA	OB1-CB1-CB2-CB3
31	A	412	SQD	C35-C36-C37-C38
47	S	620	LUT	C5-C6-C7-C8
28	C	505	CLA	C5-C6-C7-C8
28	c	503	CLA	C5-C6-C7-C8
28	G	603	CLA	CAA-CBA-CGA-O1A
28	b	603	CLA	CAA-CBA-CGA-O1A
36	S	626	3PH	O22-C21-C22-C23
31	A	412	SQD	C12-C13-C14-C15
36	t	101	3PH	C2C-C2D-C2E-C2F
28	D	402	CLA	CAA-CBA-CGA-O1A
37	j	101	DGA	OB1-CB1-CB2-CB3
28	B	606	CLA	C5-C6-C7-C8
35	c	519	DGD	C5B-C6B-C7B-C8B
45	K	101	4RF	O23-C22-C24-C25
28	c	506	CLA	C4-C3-C5-C6
46	G	601	CHL	C2-C3-C5-C6
28	B	612	CLA	C16-C17-C18-C19
28	C	503	CLA	CAD-CBD-CGD-O1D
28	G	611	CLA	CAD-CBD-CGD-O1D
28	S	604	CLA	CAD-CBD-CGD-O1D
28	b	605	CLA	CAD-CBD-CGD-O1D
28	b	615	CLA	CAD-CBD-CGD-O1D
31	A	412	SQD	O5-C5-C6-S
31	b	626	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
35	B	623	DGD	C3G-C2G-O2G-C1B
35	b	623	DGD	C3G-C2G-O2G-C1B
39	c	527	LMK	C29-C28-O8-C9
46	Y	609	CHL	CAD-CBD-CGD-O1D
51	Y	626	PTY	C2-C3-O11-P1
51	Y	627	PTY	C2-C3-O11-P1
32	C	523	LMG	O9-C10-C11-C12
46	G	605	CHL	CAA-CBA-CGA-O1A
35	C	519	DGD	C3B-C4B-C5B-C6B
36	b	624	3PH	C26-C27-C28-C29
38	L	101	LHG	C17-C18-C19-C20
32	c	523	LMG	O8-C28-C29-C30
37	C	524	DGA	OG2-CB1-CB2-CB3
28	S	610	CLA	C5-C6-C7-C8
28	c	509	CLA	C13-C15-C16-C17
28	C	502	CLA	C6-C7-C8-C9
46	Y	601	CHL	C11-C12-C13-C14
38	C	525	LHG	C31-C32-C33-C34
32	C	523	LMG	C34-C35-C36-C37
32	w	201	LMG	O9-C10-C11-C12
28	B	606	CLA	CAA-CBA-CGA-O2A
28	N	611	CLA	CAA-CBA-CGA-O2A
28	b	609	CLA	CAA-CBA-CGA-O2A
35	C	518	DGD	O2G-C1B-C2B-C3B
38	S	624	LHG	O8-C23-C24-C25
38	d	409	LHG	C11-C10-C9-C8
28	b	615	CLA	CAA-CBA-CGA-O1A
36	B	624	3PH	C2E-C2F-C2G-C2H
28	G	602	CLA	C15-C16-C17-C18
28	c	505	CLA	CAA-CBA-CGA-O2A
28	c	512	CLA	CAA-CBA-CGA-O2A
32	B	622	LMG	O7-C10-C11-C12
37	J	101	DGA	OG2-CB1-CB2-CB3
37	c	524	DGA	OG1-CA1-CA2-CA3
28	b	613	CLA	C8-C10-C11-C12
38	D	408	LHG	C35-C36-C37-C38
32	W	201	LMG	O9-C10-C11-C12
38	d	409	LHG	O9-C7-C8-C9
38	G	624	LHG	C34-C35-C36-C37
28	b	606	CLA	C13-C15-C16-C17
28	B	612	CLA	C6-C7-C8-C10
28	D	403	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
28	S	602	CLA	C11-C10-C8-C7
28	Y	602	CLA	C11-C12-C13-C15
28	b	604	CLA	C2-C3-C5-C6
28	b	615	CLA	C11-C12-C13-C15
28	c	512	CLA	C12-C13-C15-C16
45	I	102	4RF	C41-C43-C44-C45
46	N	609	CHL	C12-C13-C15-C16
46	G	601	CHL	C11-C12-C13-C15
28	B	608	CLA	CAA-CBA-CGA-O1A
31	b	621	SQD	O49-C7-C8-C9
35	c	518	DGD	O1B-C1B-C2B-C3B
37	C	524	DGA	OB1-CB1-CB2-CB3
37	B	625	DGA	CBA-CCA-CDA-CEA
28	C	503	CLA	CAA-CBA-CGA-O2A
28	C	505	CLA	CAA-CBA-CGA-O2A
28	b	608	CLA	CAA-CBA-CGA-O2A
28	b	613	CLA	CAA-CBA-CGA-O2A
31	a	412	SQD	O47-C7-C8-C9
35	c	518	DGD	O2G-C1B-C2B-C3B
38	D	409	LHG	O7-C7-C8-C9
38	Y	624	LHG	O8-C23-C24-C25
37	j	101	DGA	CBB-CAB-CB9-CB8
38	D	410	LHG	C29-C30-C31-C32
38	L	101	LHG	C12-C13-C14-C15
32	D	411	LMG	C10-C11-C12-C13
30	c	516	BCR	C17-C18-C19-C20
28	A	406	CLA	CAA-CBA-CGA-O1A
28	N	614	CLA	CAA-CBA-CGA-O1A
28	b	613	CLA	CAA-CBA-CGA-O1A
28	c	505	CLA	CAA-CBA-CGA-O1A
35	C	518	DGD	O1B-C1B-C2B-C3B
37	b	625	DGA	OA1-CA1-CA2-CA3
47	G	621	LUT	C9-C10-C11-C12
33	A	414	SPH	C14-C15-C16-C17
28	Y	614	CLA	C16-C17-C18-C20
28	b	615	CLA	C16-C17-C18-C19
28	A	406	CLA	CAA-CBA-CGA-O2A
31	a	412	SQD	C32-C33-C34-C35
28	B	603	CLA	C8-C10-C11-C12
28	B	607	CLA	C5-C6-C7-C8
28	c	504	CLA	C8-C10-C11-C12
28	d	402	CLA	C5-C6-C7-C8

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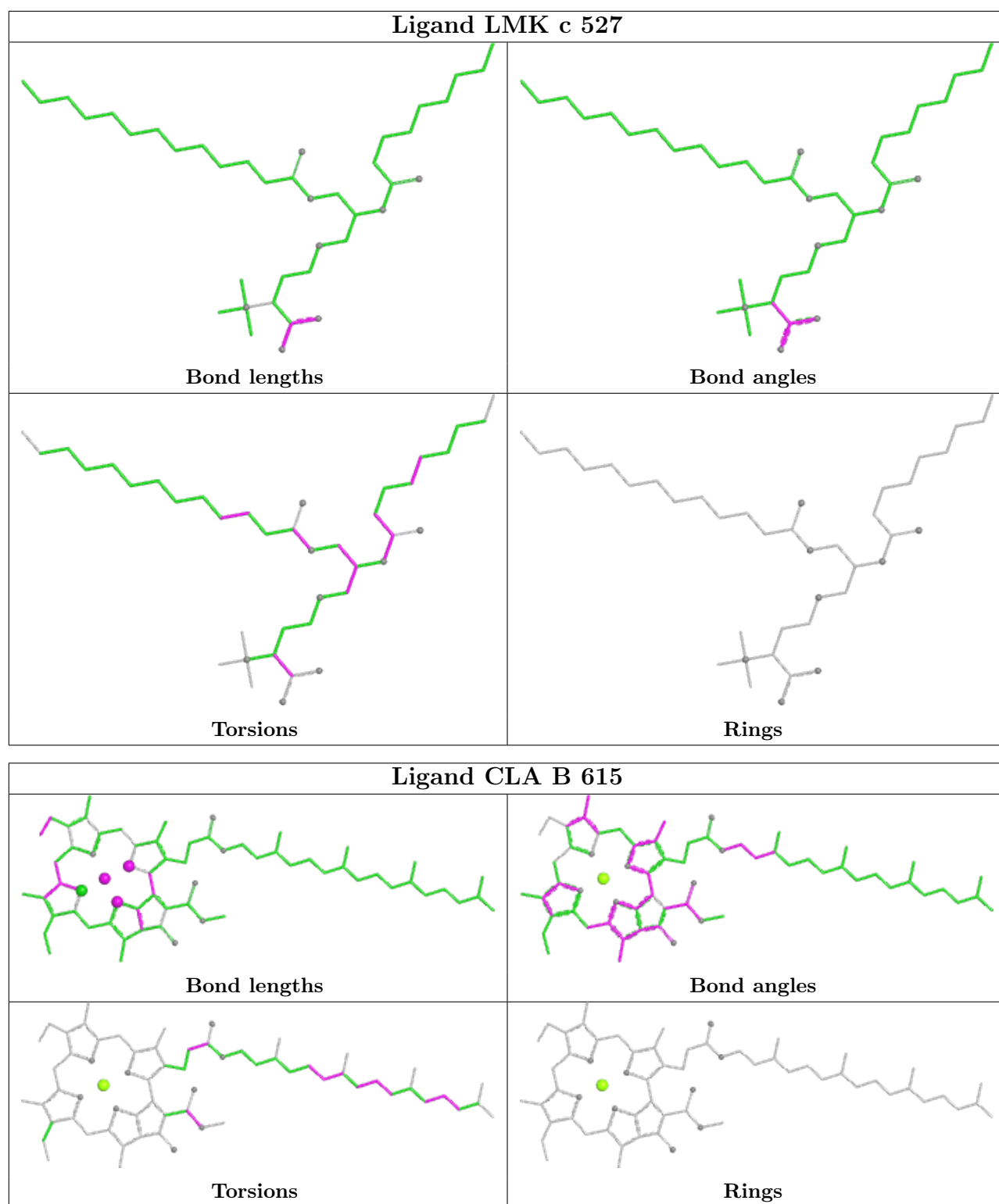
Mol	Chain	Res	Type	Atoms
38	d	410	LHG	C34-C35-C36-C37
51	Y	626	PTY	C13-C14-C15-C16
28	C	503	CLA	CAA-CBA-CGA-O1A
28	G	614	CLA	CAA-CBA-CGA-O1A
28	b	609	CLA	CAA-CBA-CGA-O1A
28	c	512	CLA	CAA-CBA-CGA-O1A
38	S	624	LHG	O10-C23-C24-C25
38	Y	624	LHG	O10-C23-C24-C25
37	c	524	DGA	CA2-CA1-OG1-CG1
38	N	624	LHG	O7-C7-C8-C9
28	N	611	CLA	CAA-CBA-CGA-O1A
28	S	610	CLA	CAA-CBA-CGA-O1A
28	D	402	CLA	C8-C10-C11-C12
28	b	612	CLA	C15-C16-C17-C18
39	c	527	LMK	C29-C30-C31-C32
28	C	508	CLA	CAA-CBA-CGA-O2A
28	C	512	CLA	CAA-CBA-CGA-O2A
37	b	625	DGA	OG2-CB1-CB2-CB3

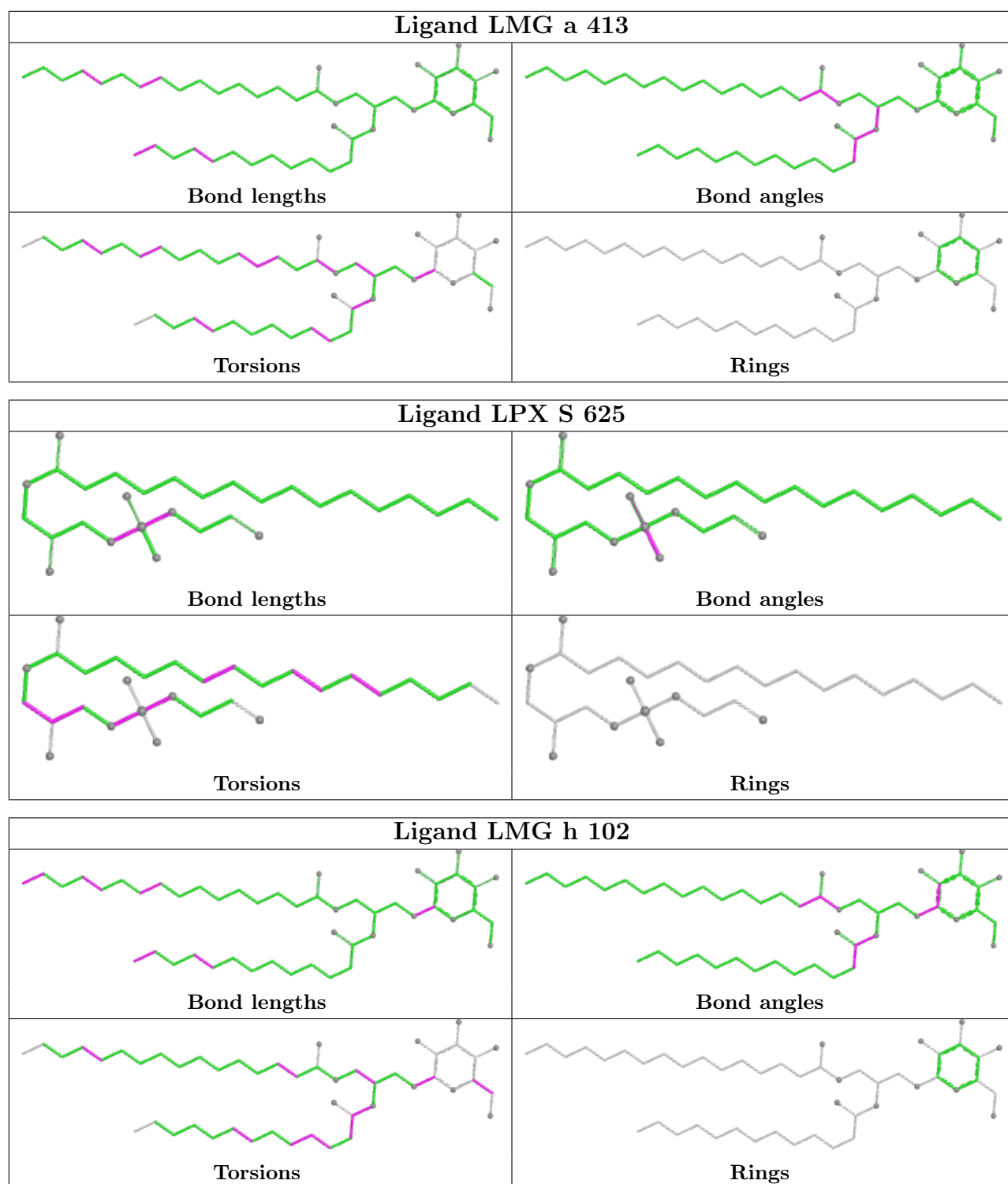
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	N	623	NEX	C1-C2-C3-C4-C5-C6

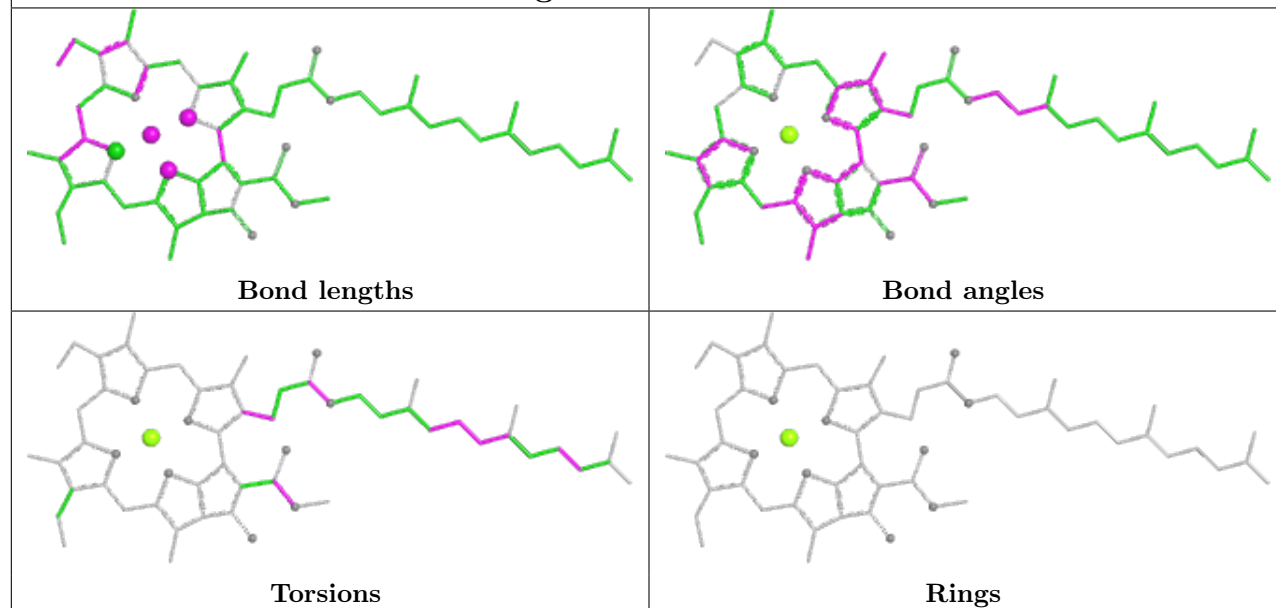
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

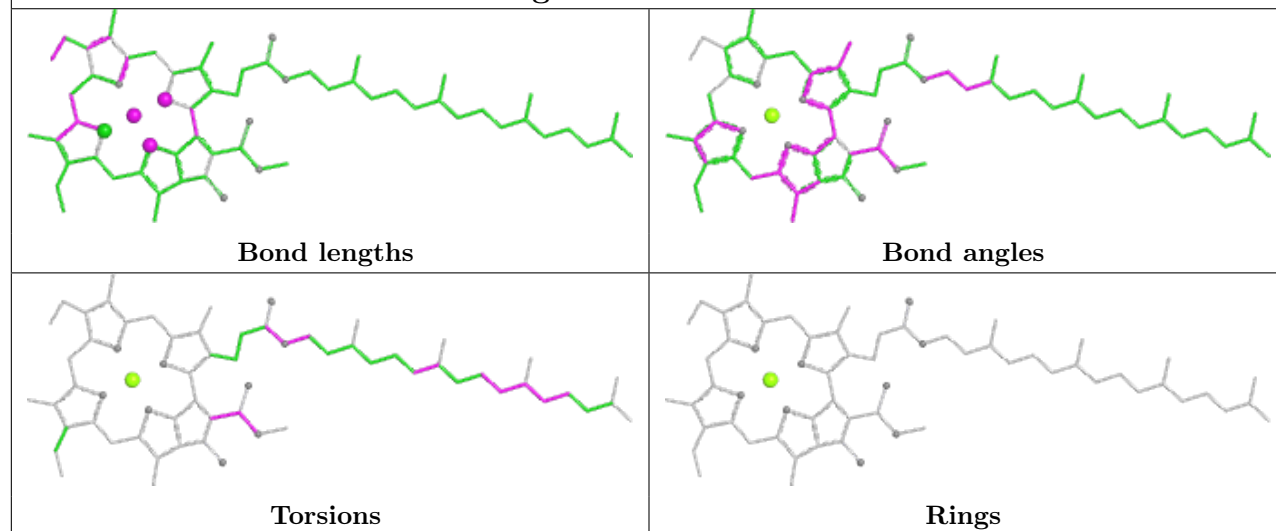


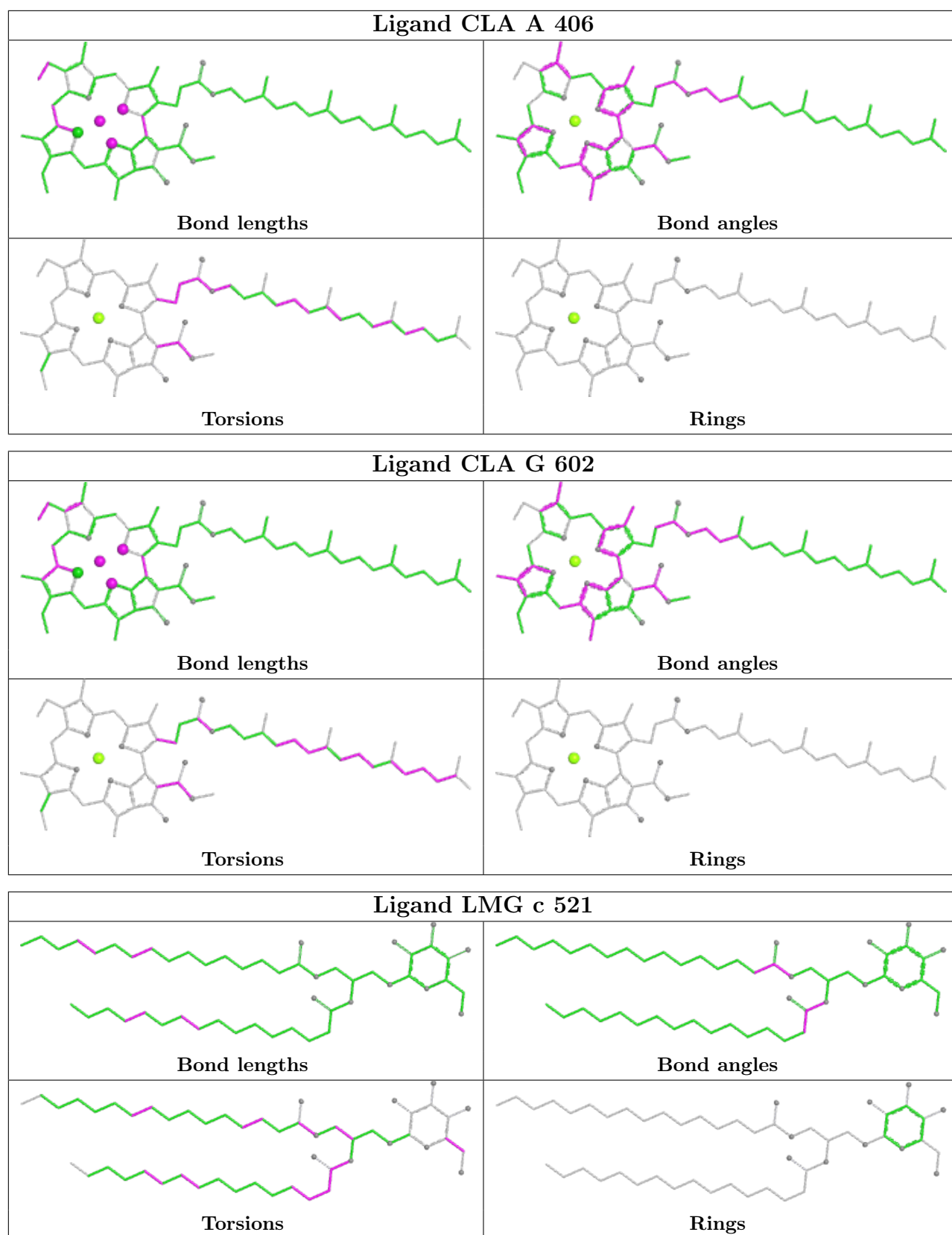


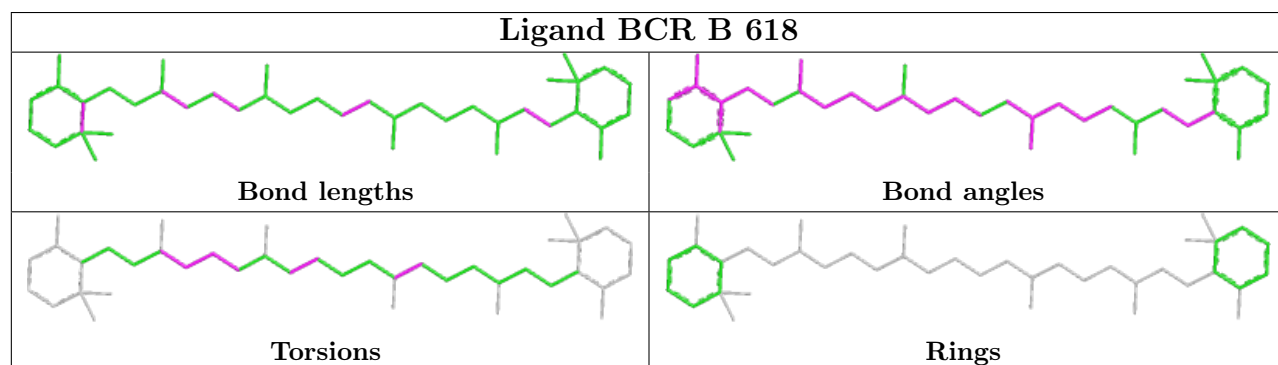
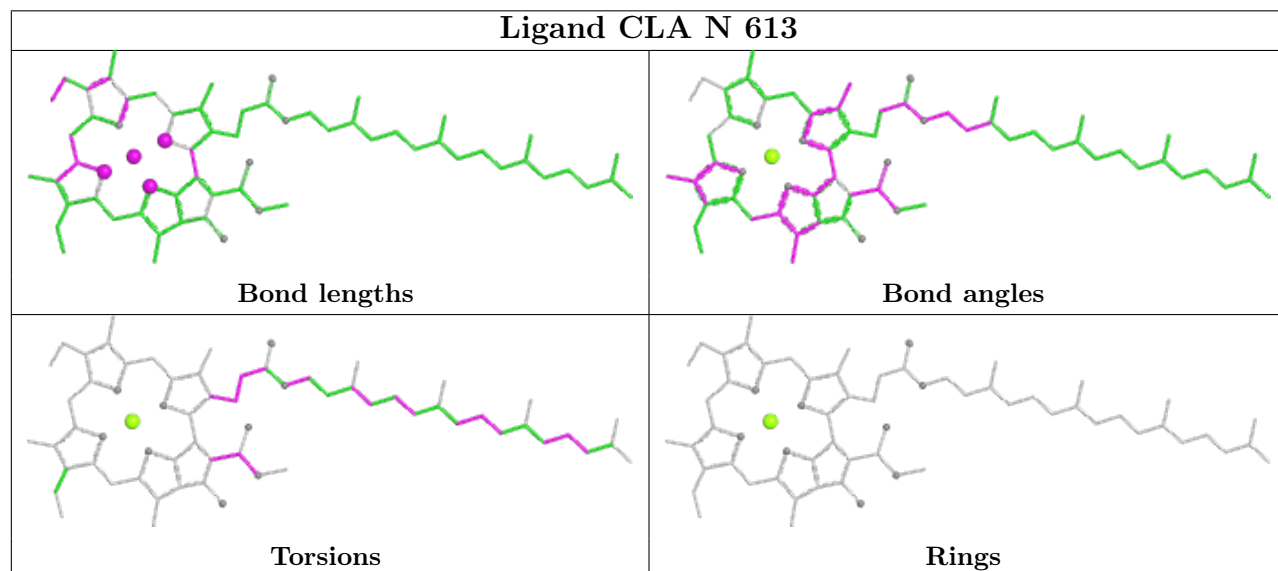
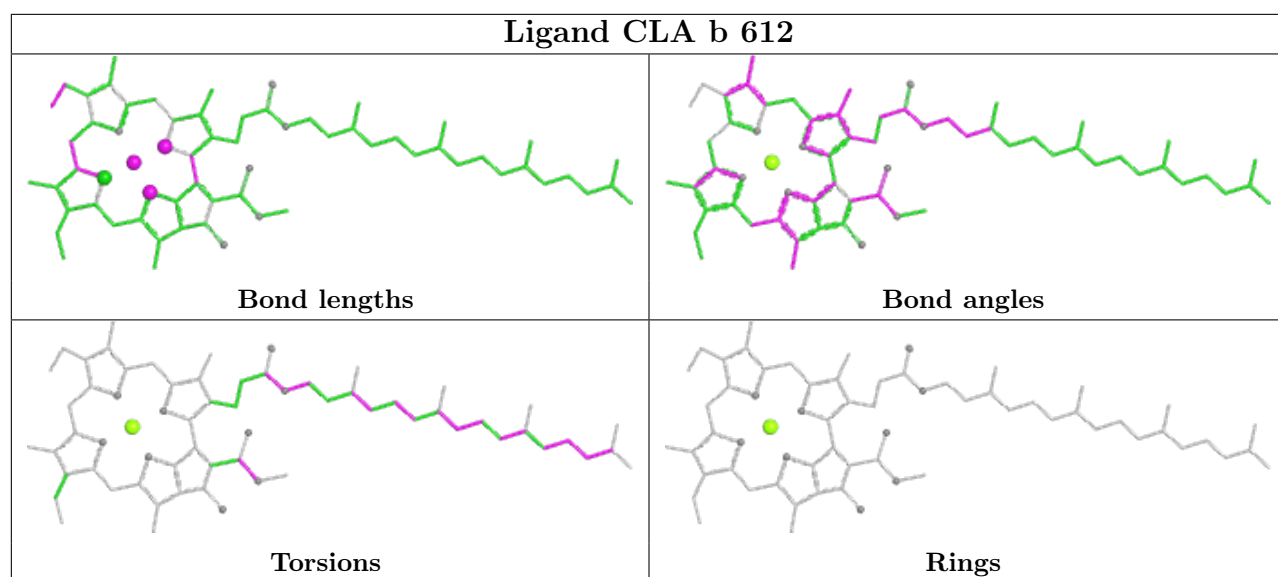
Ligand CLA S 609

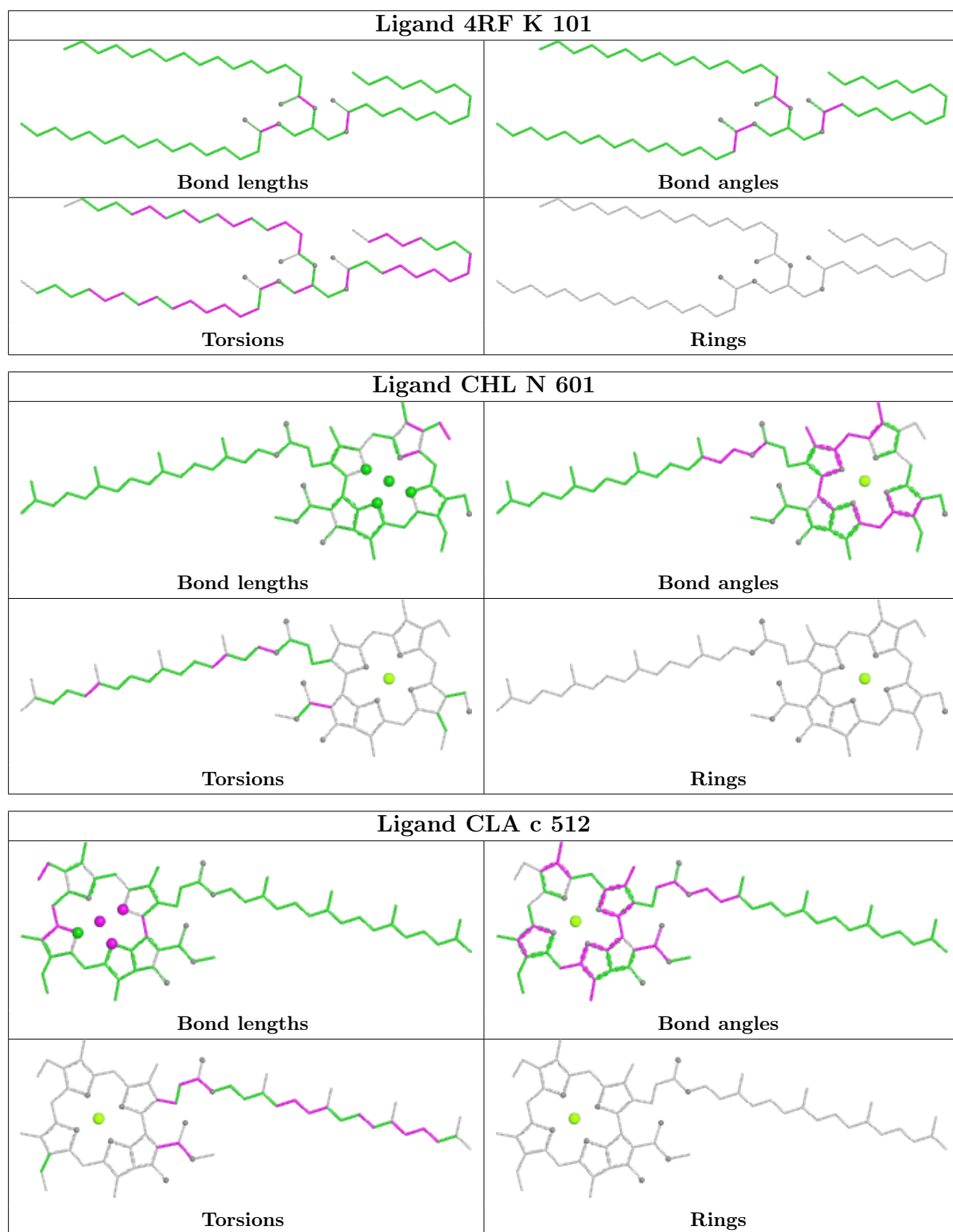


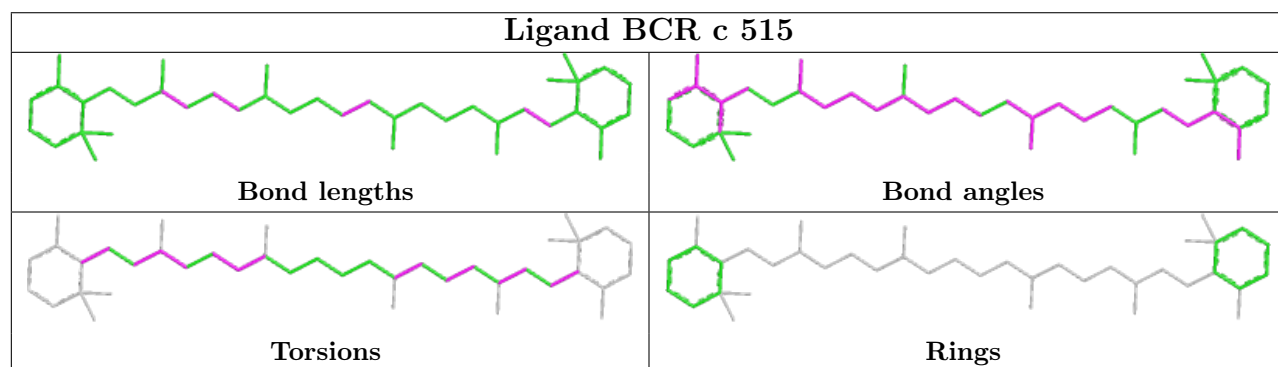
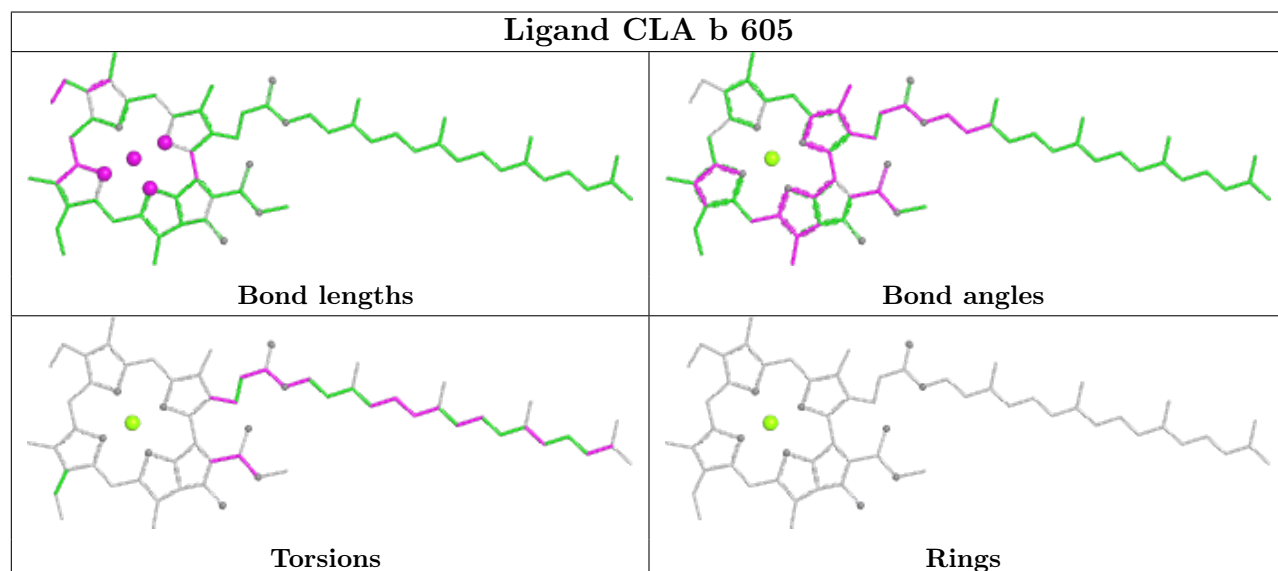
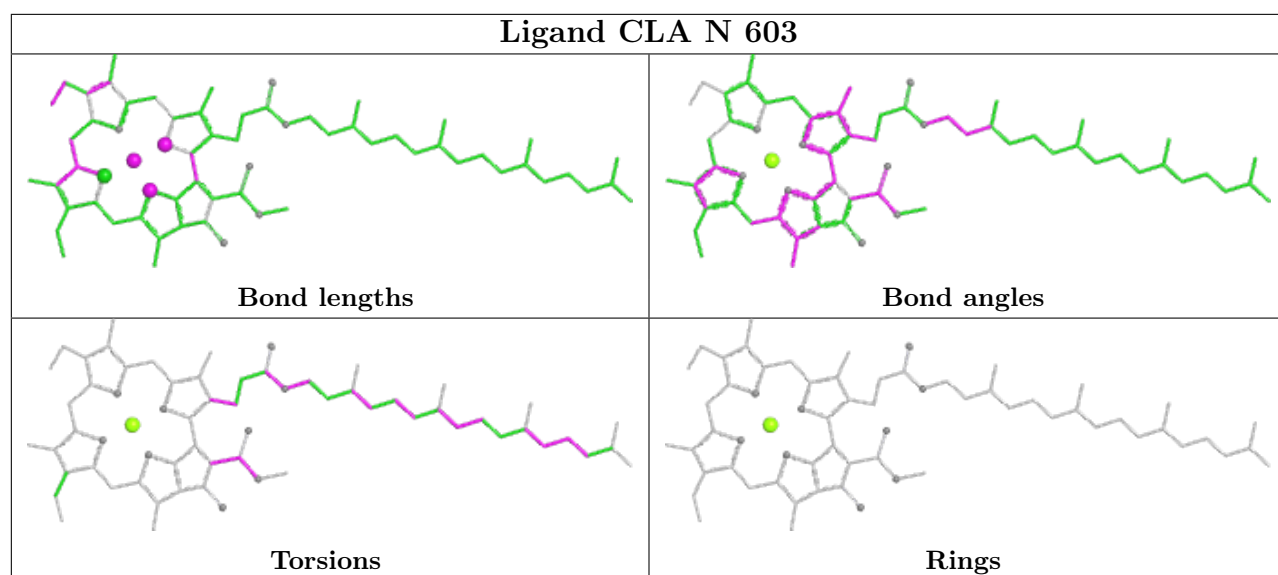
Ligand CLA B 616

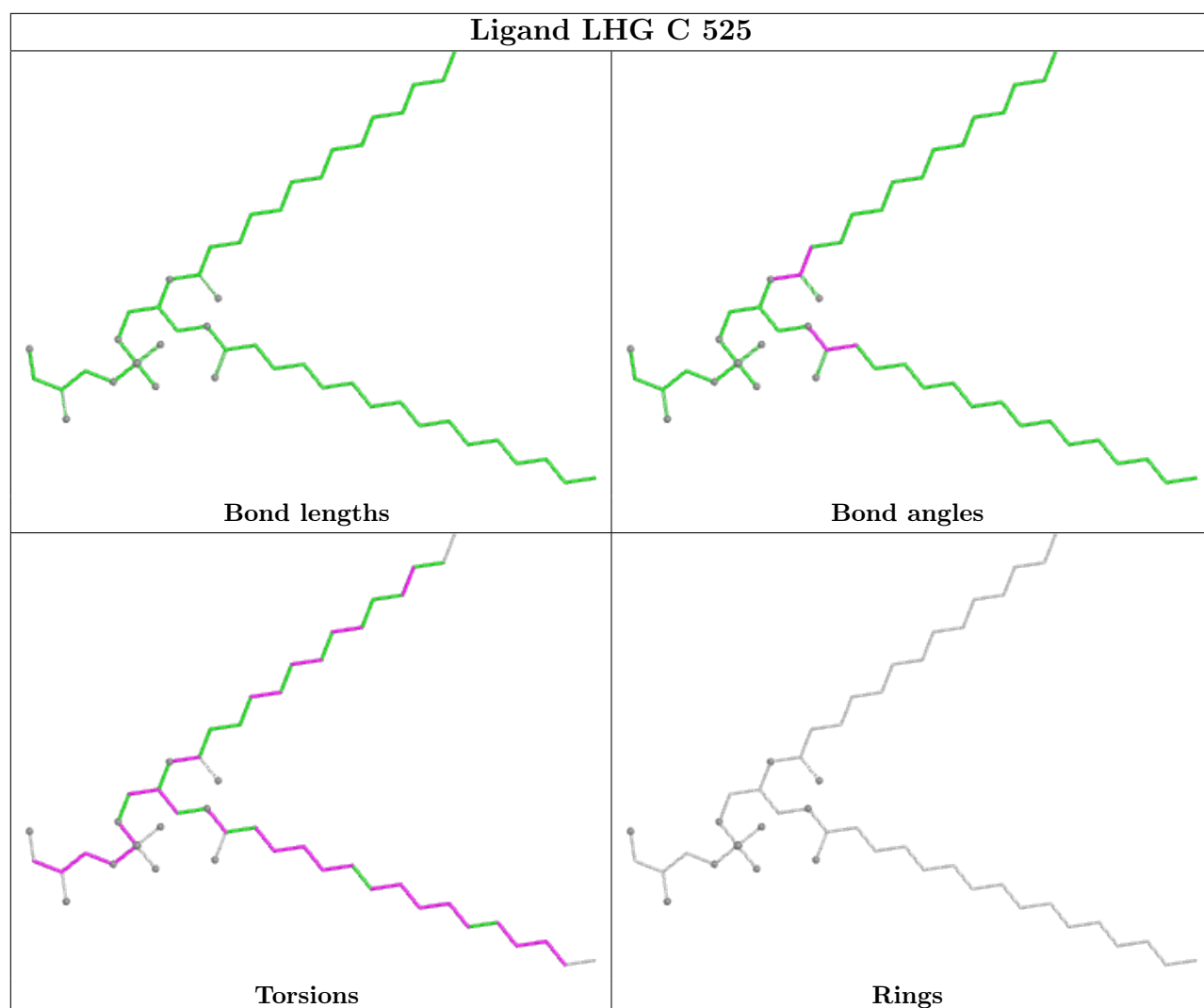


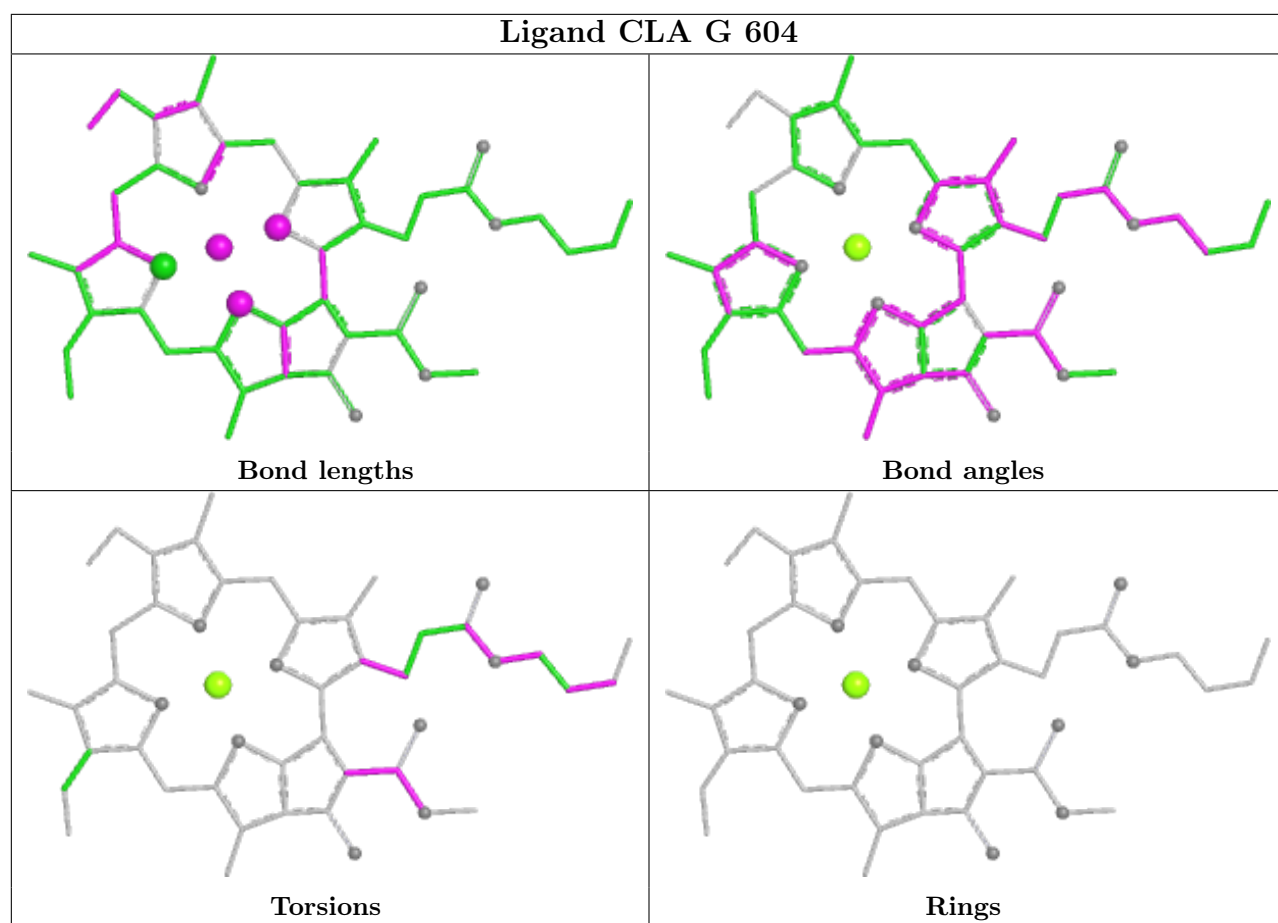


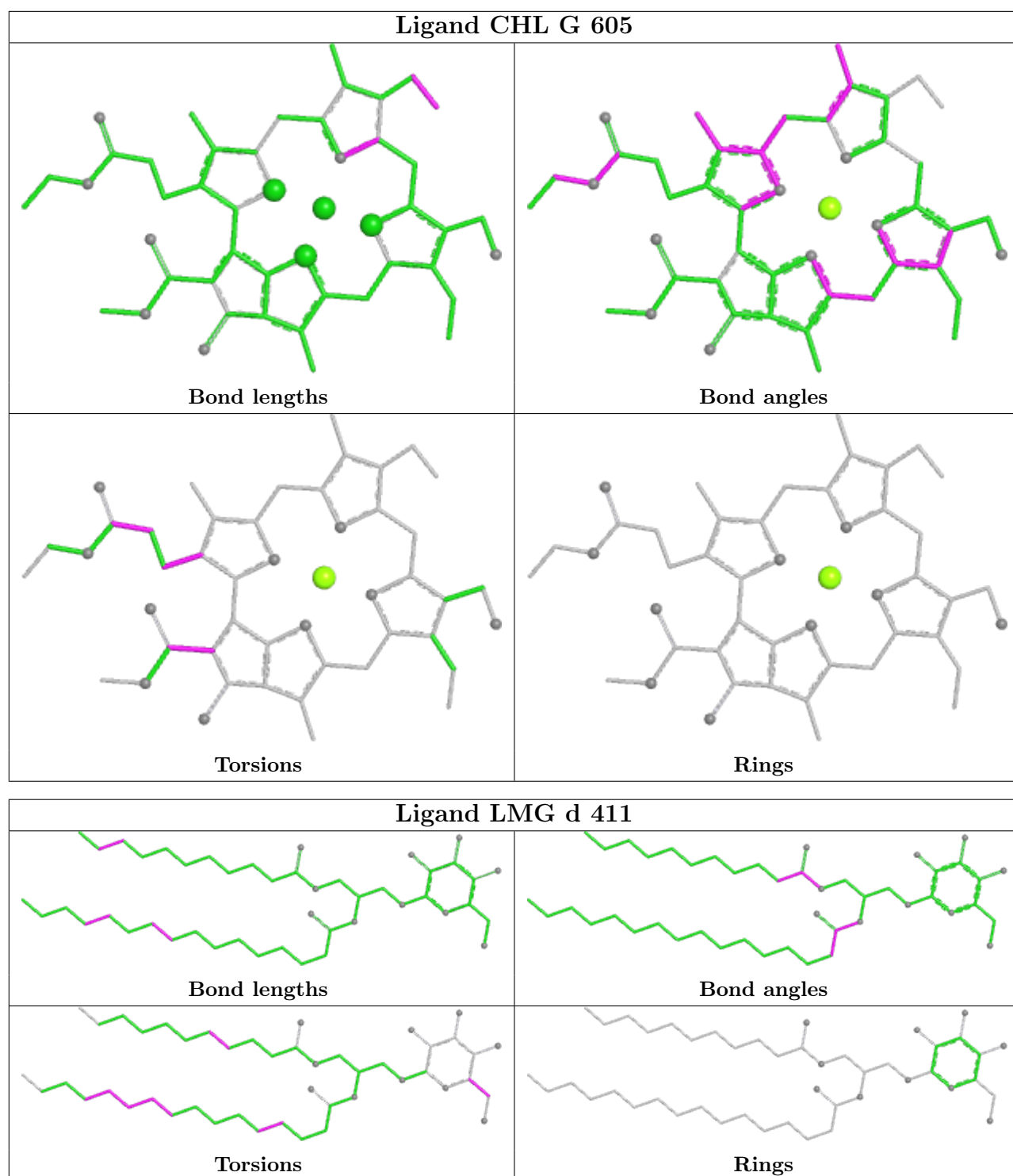


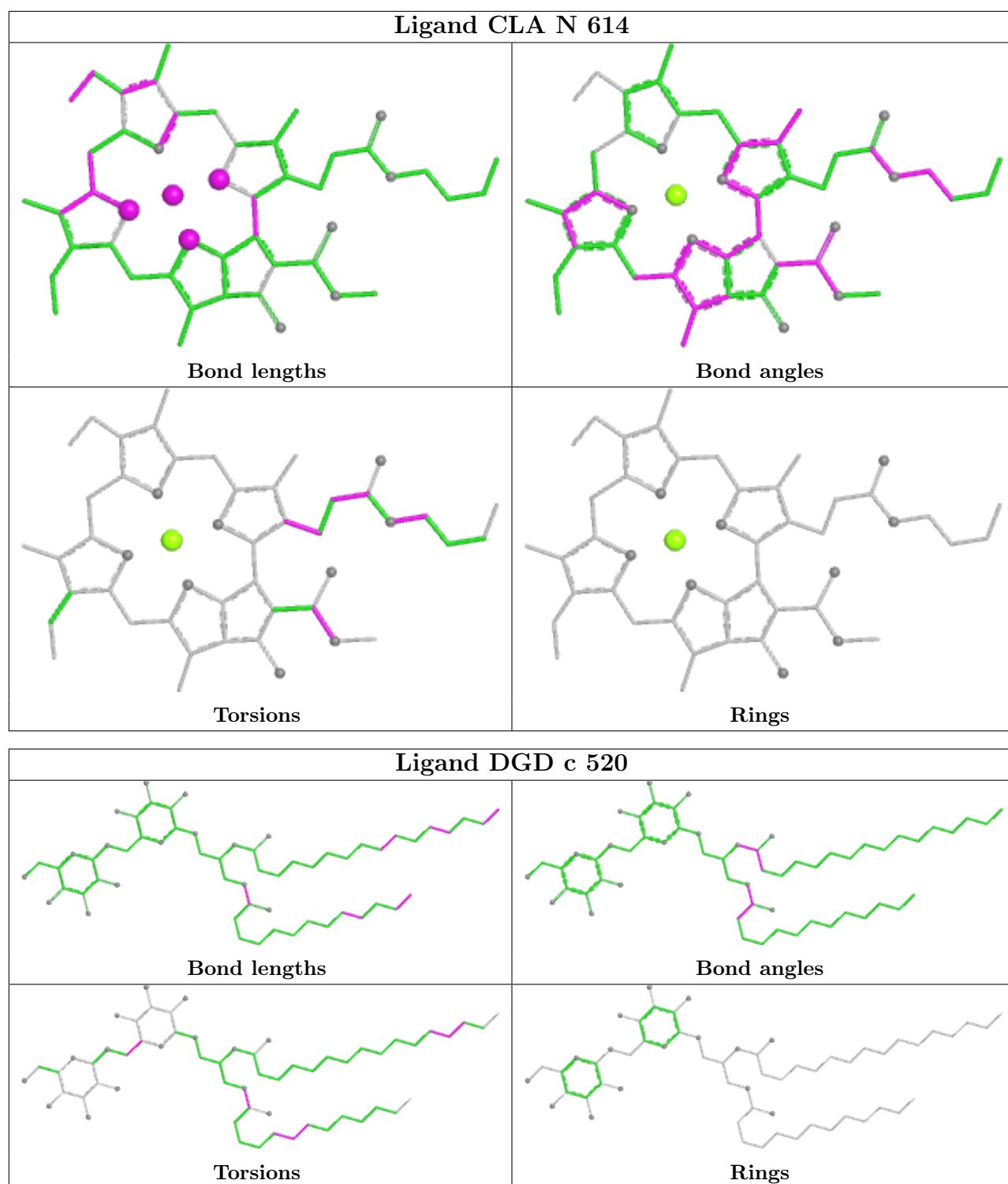


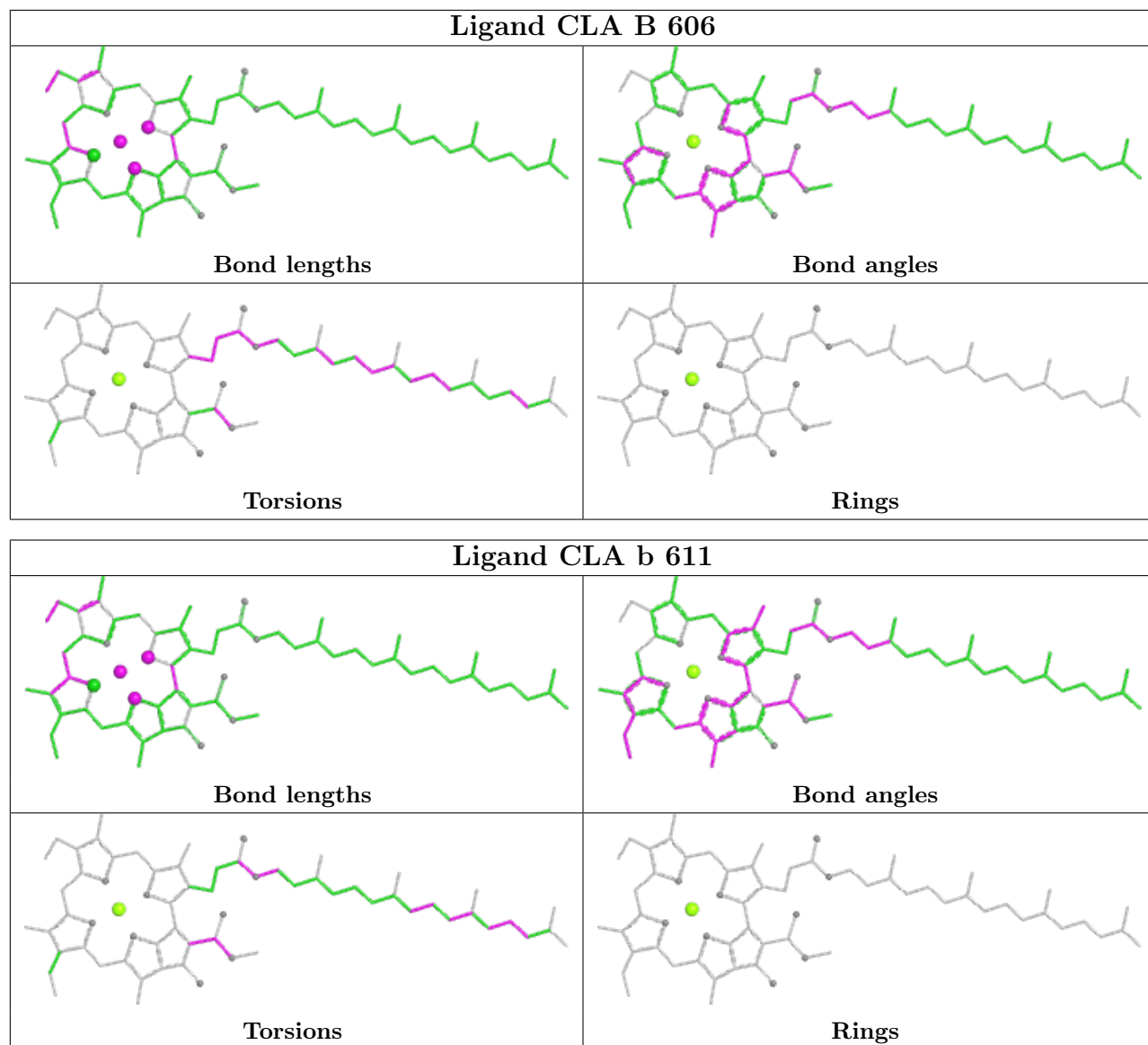


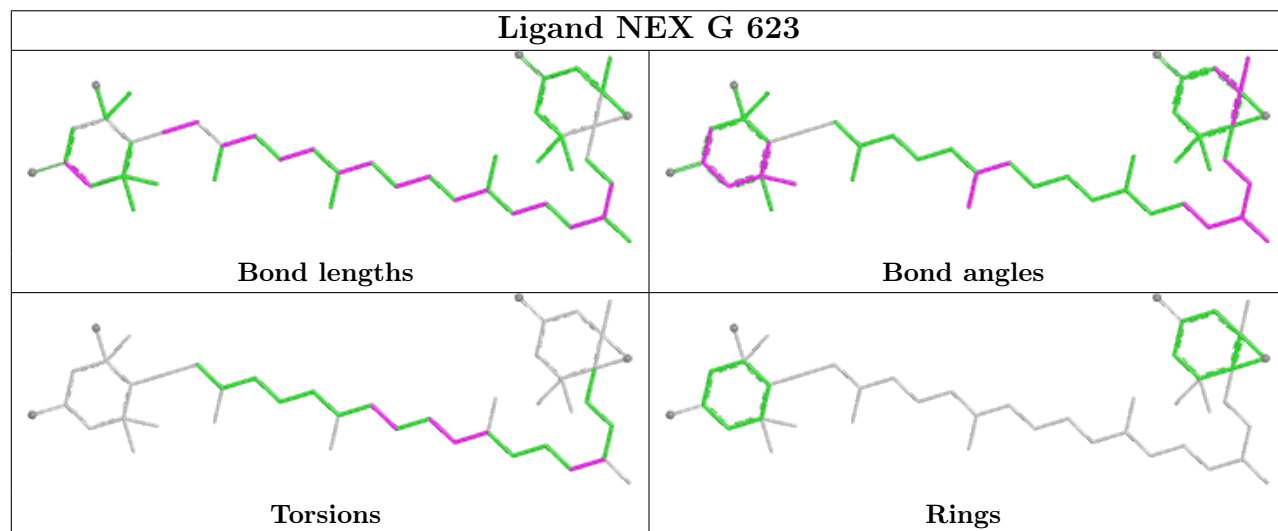
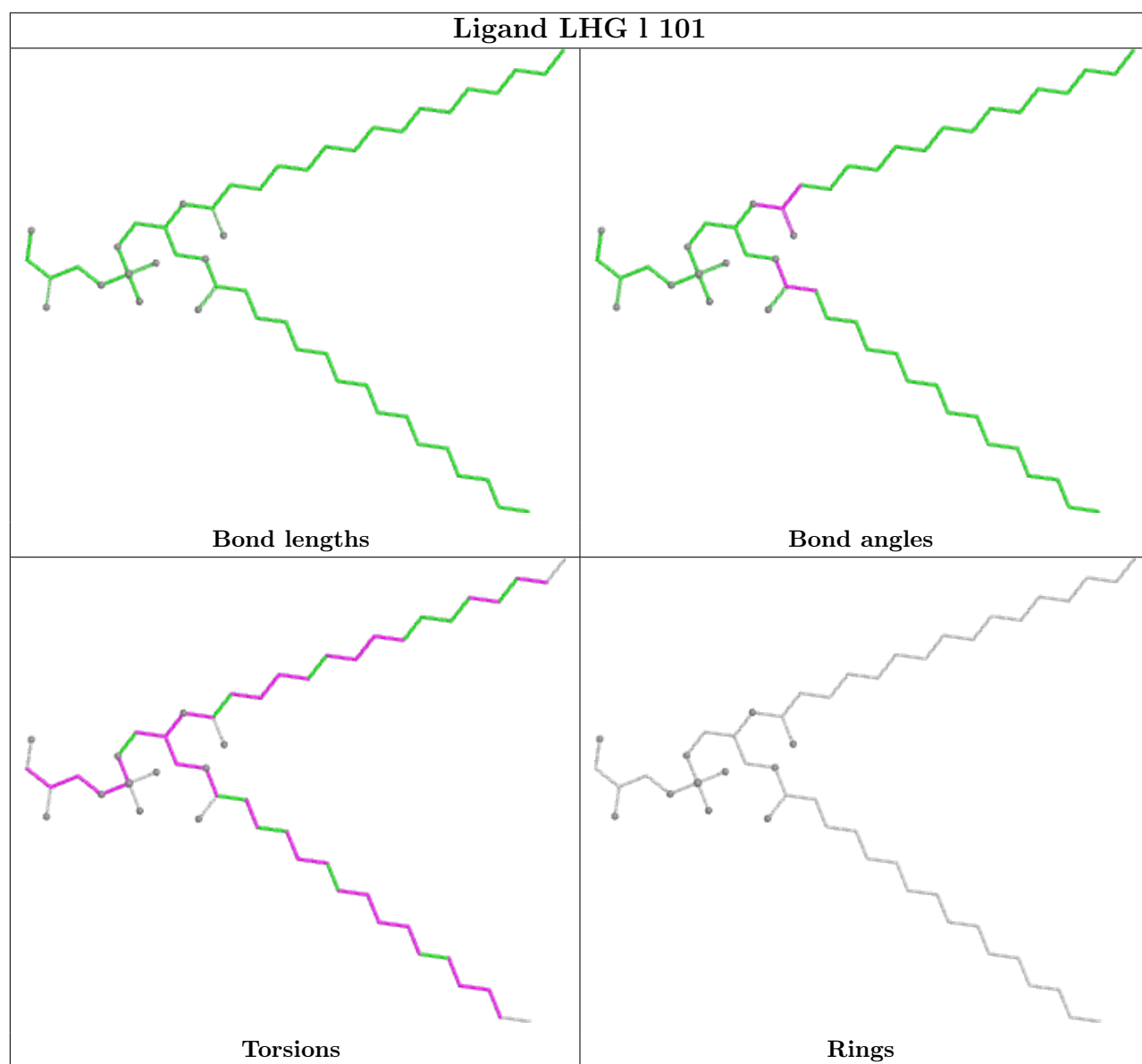


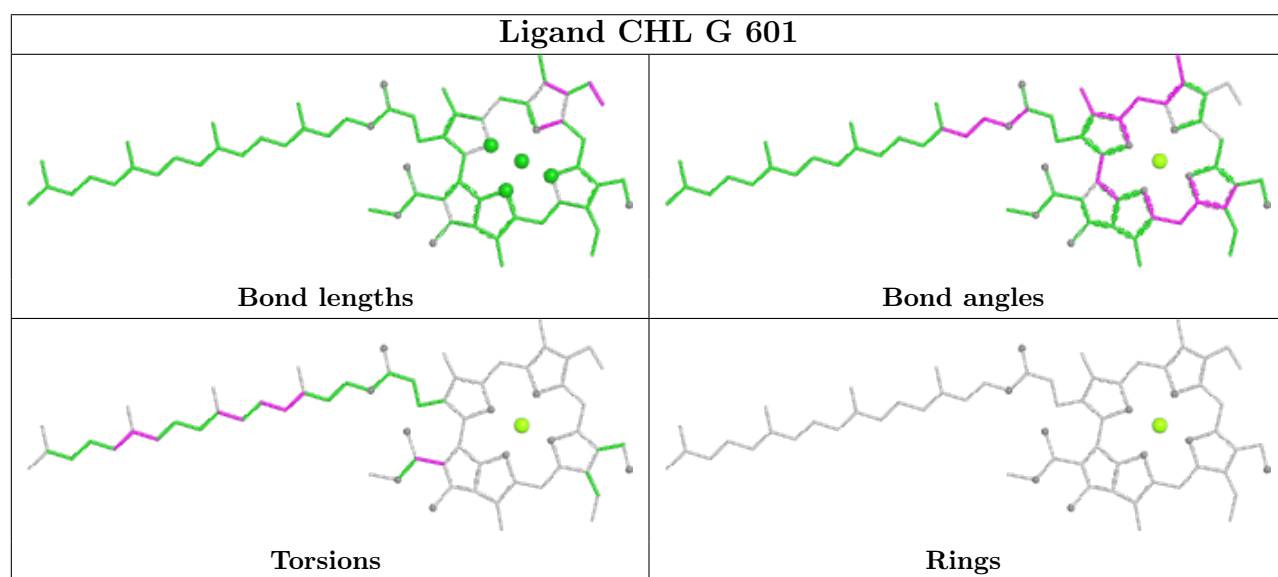
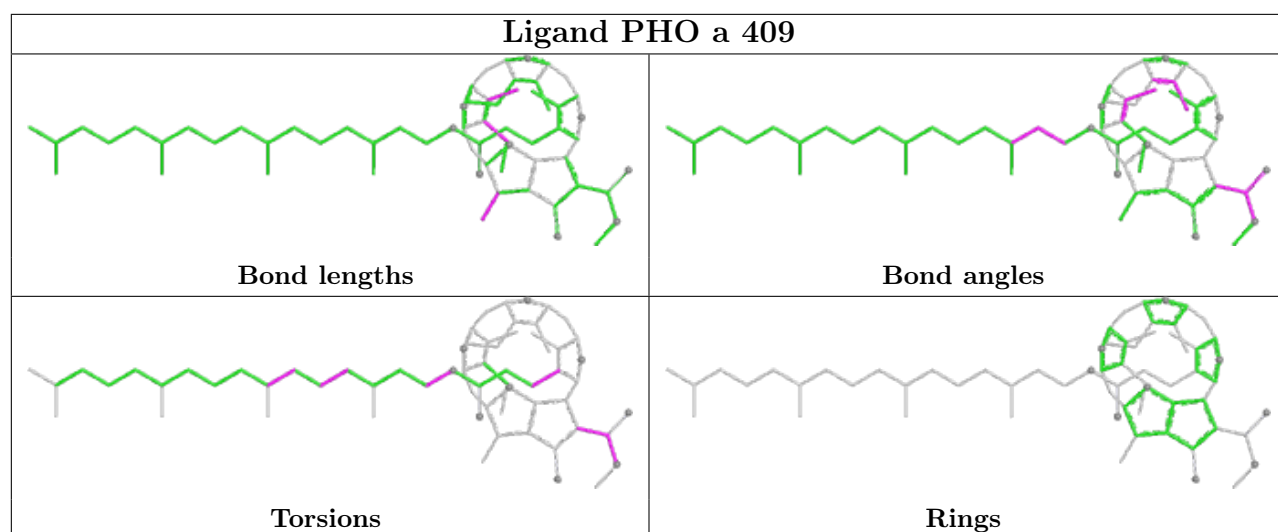


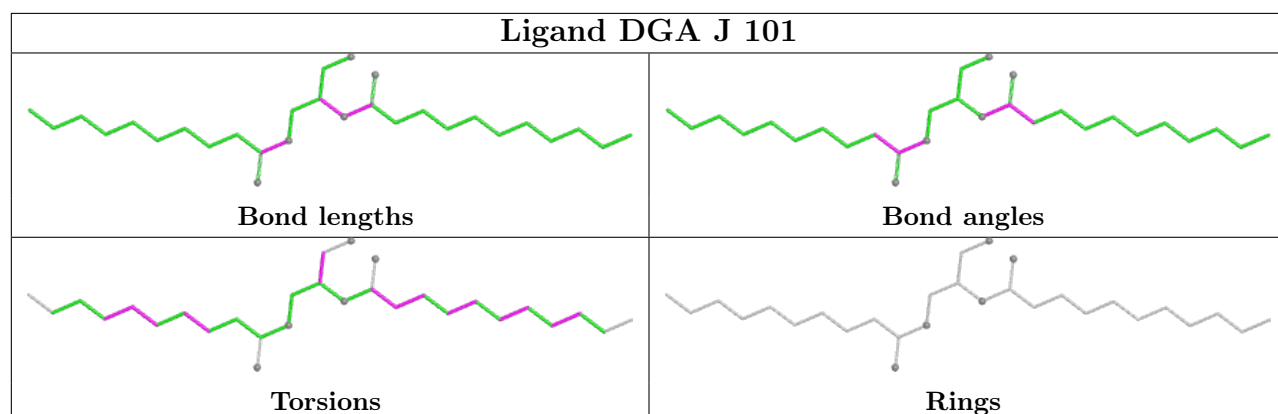
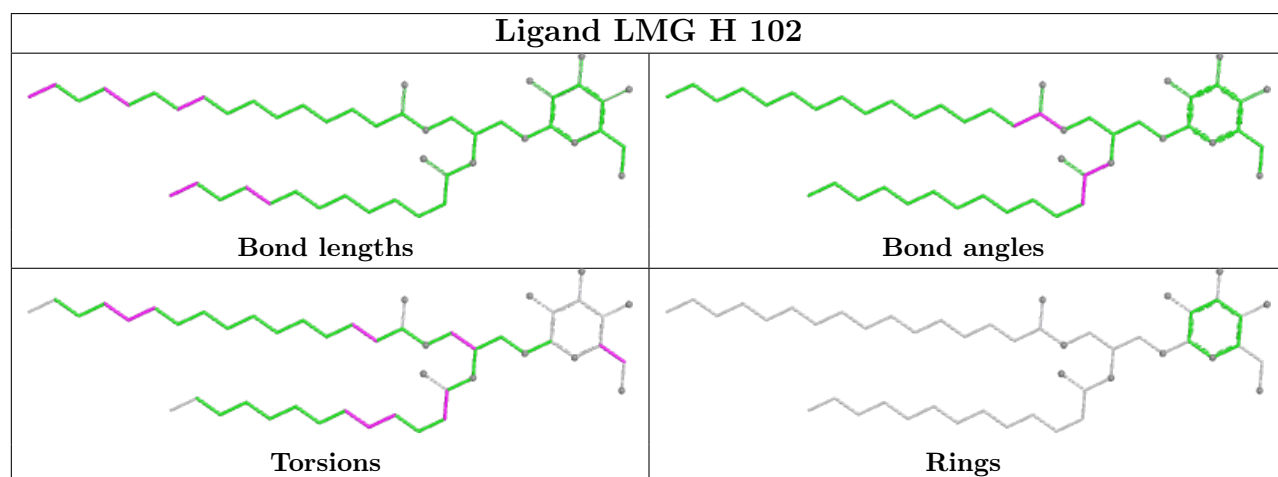
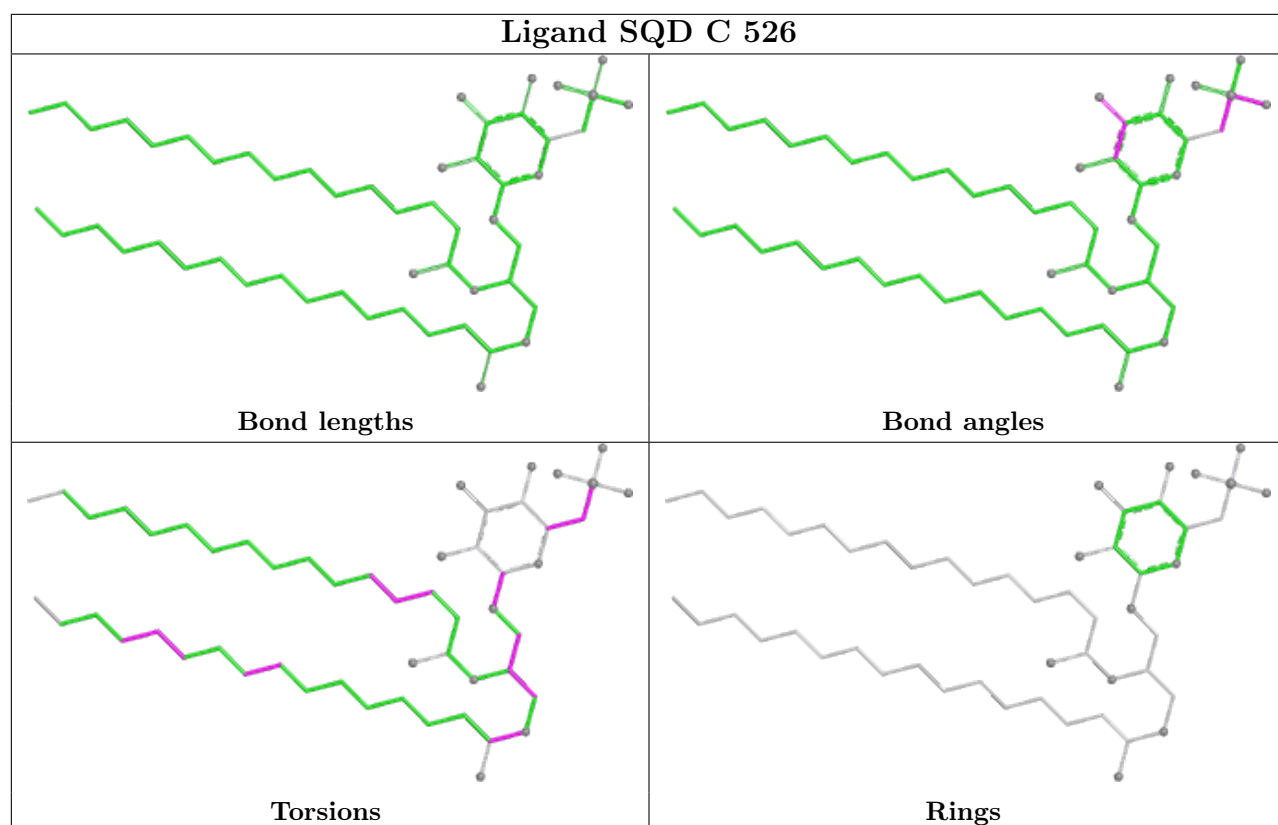


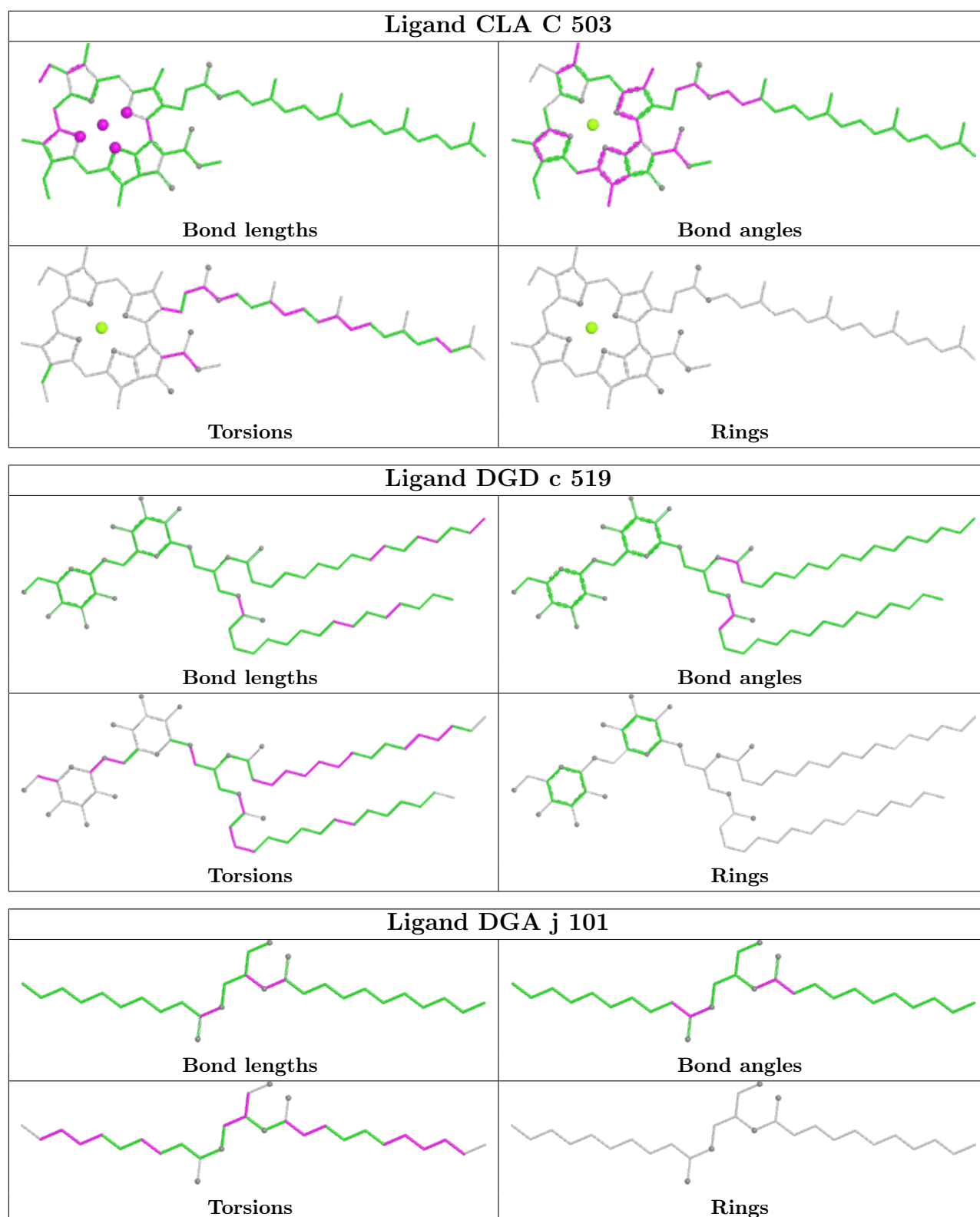


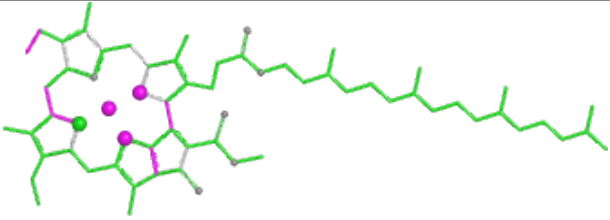
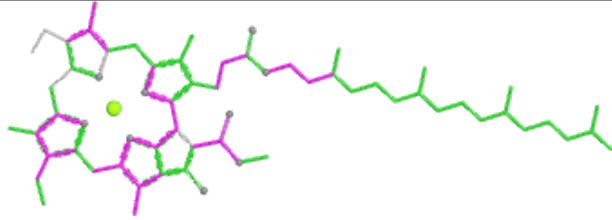
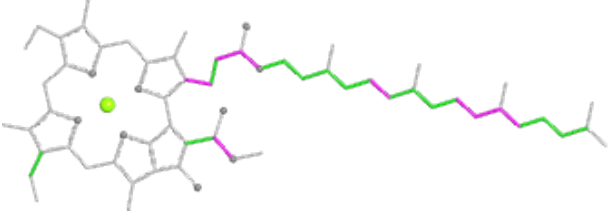
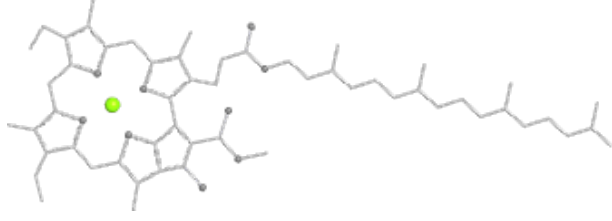
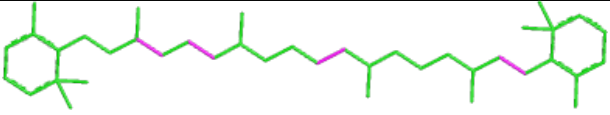
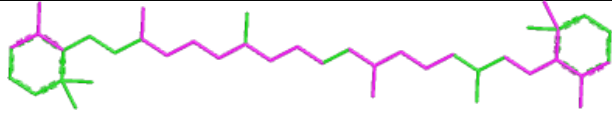
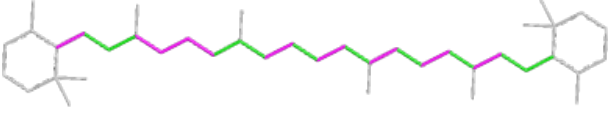
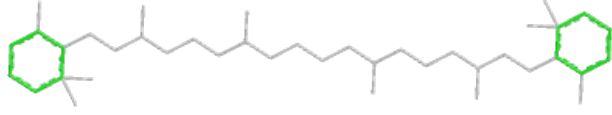
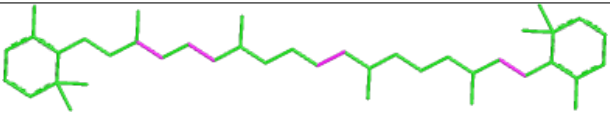
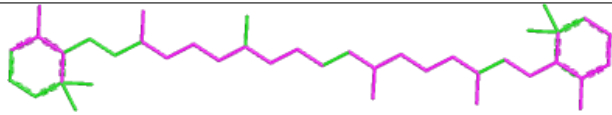
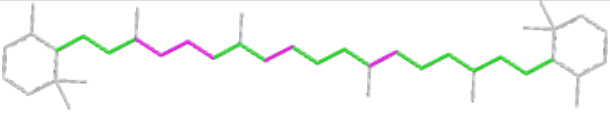



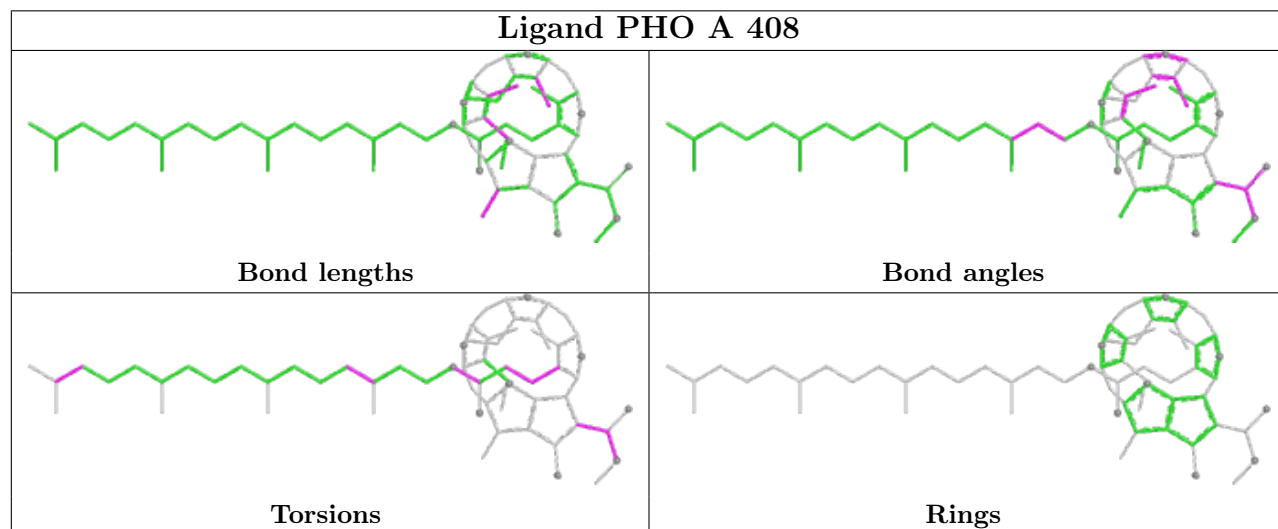
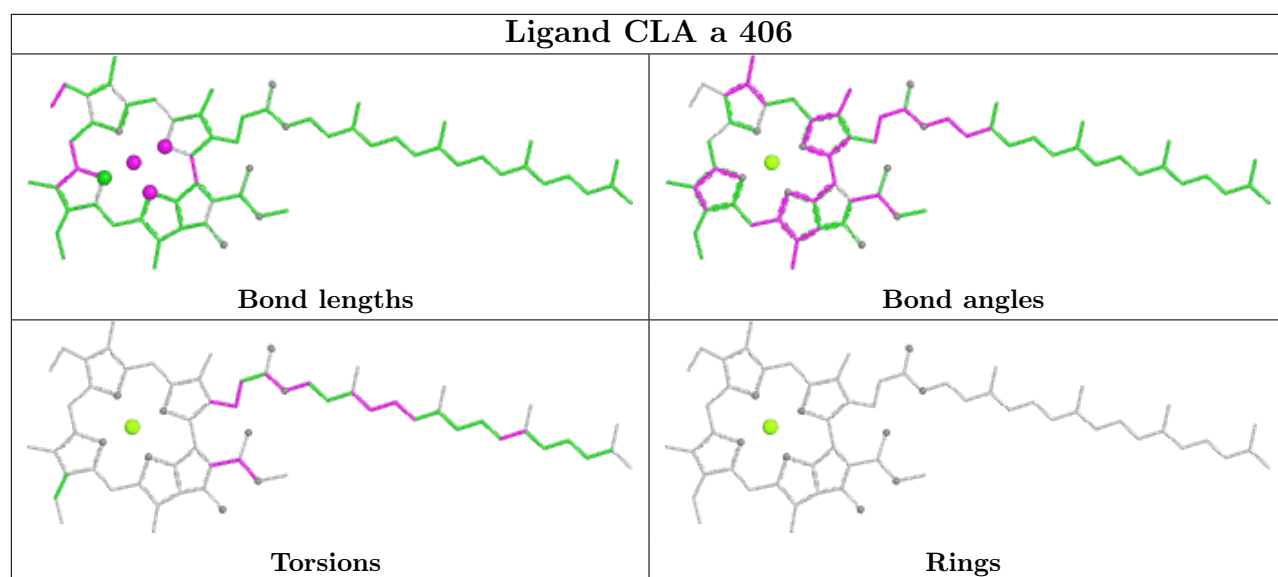




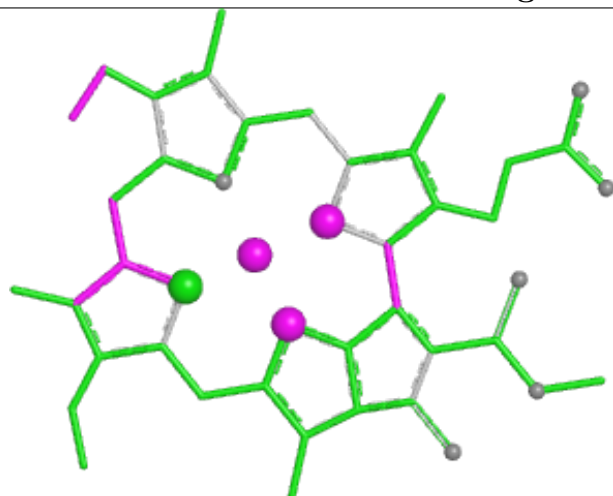




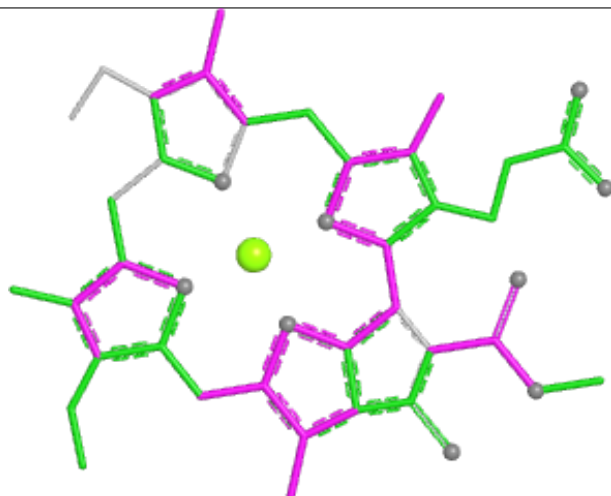
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 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR C 514	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR b 618	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



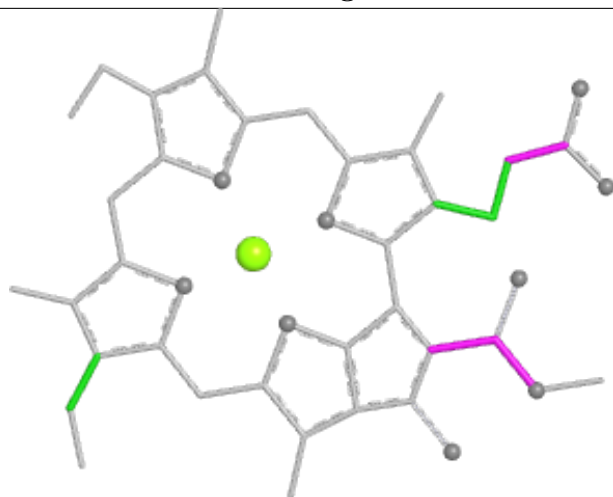
Ligand CLA S 612



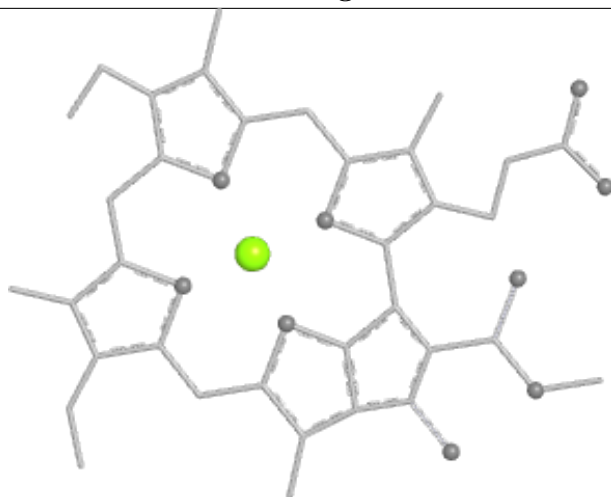
Bond lengths



Bond angles

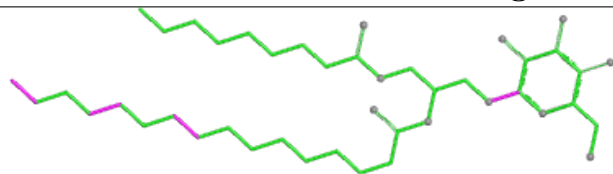


Torsions

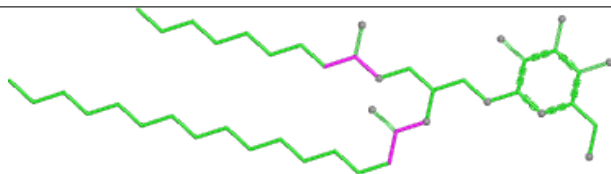


Rings

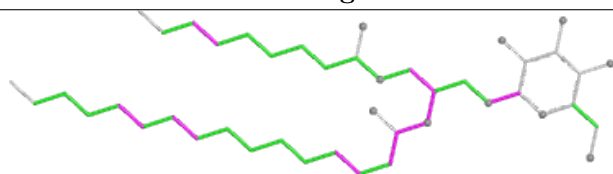
Ligand LMG B 622



Bond lengths



Bond angles

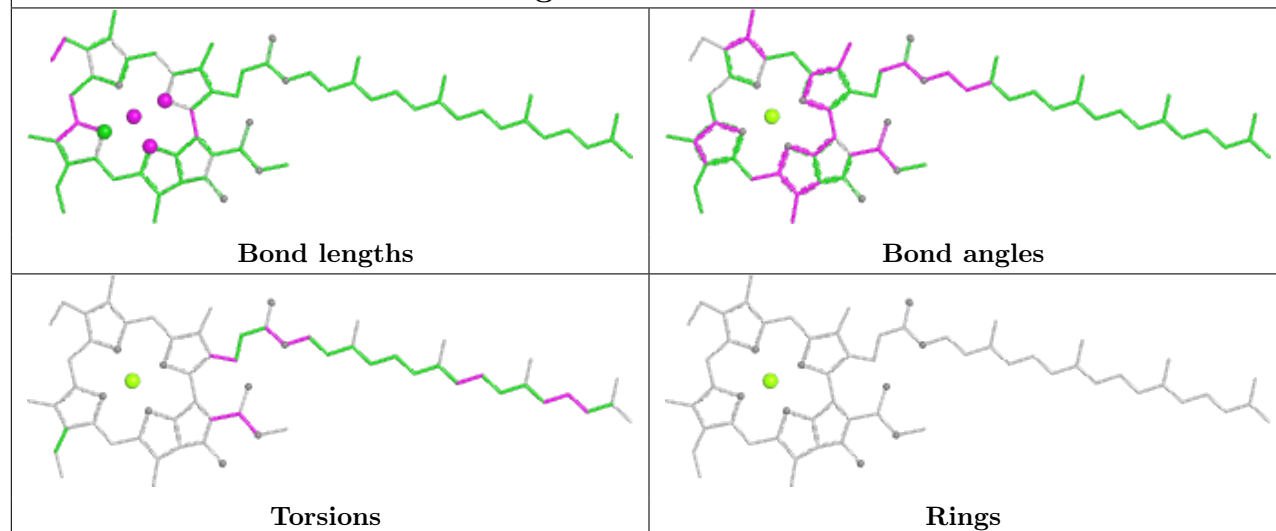


Torsions

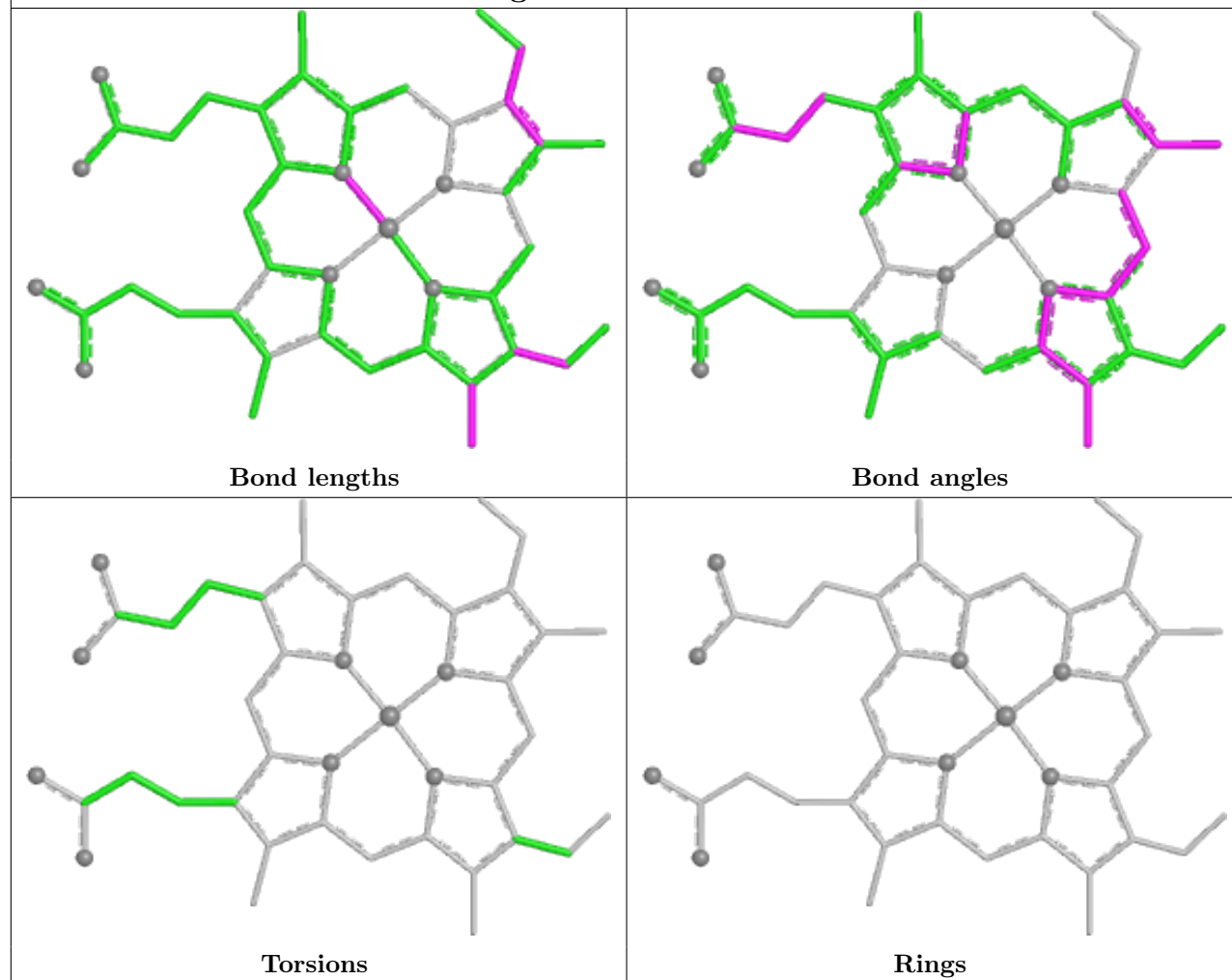


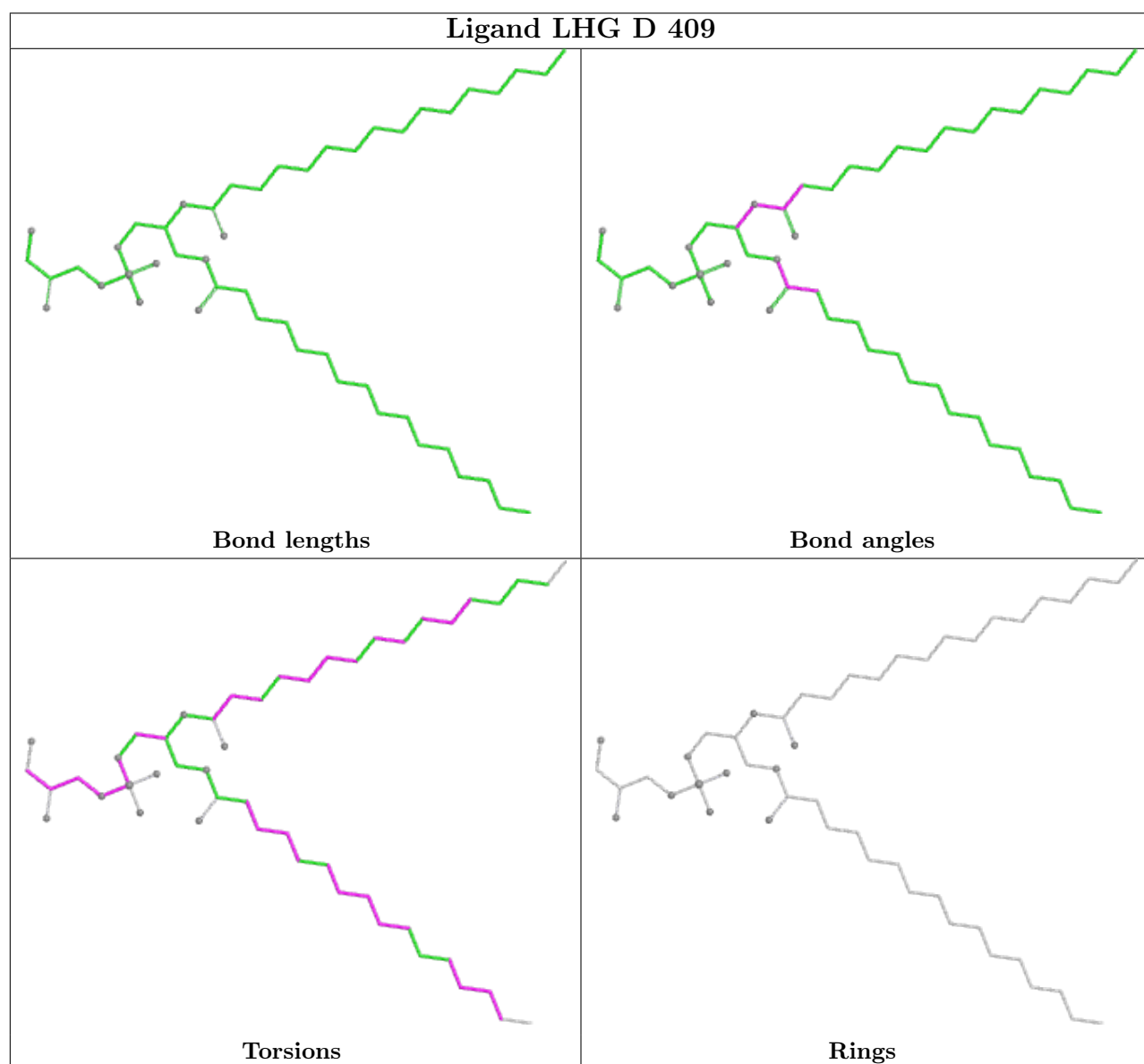
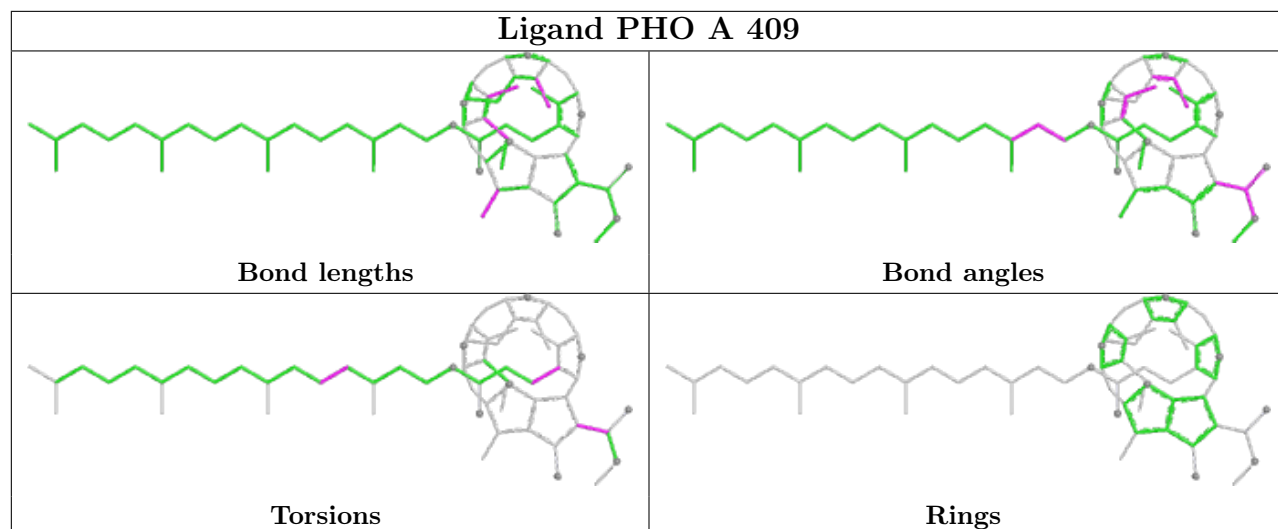
Rings

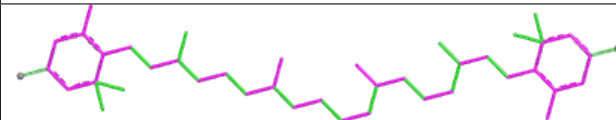
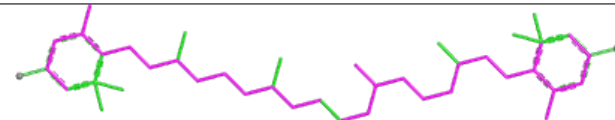
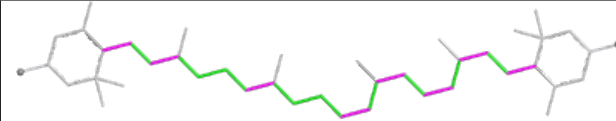
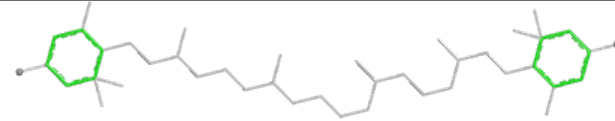
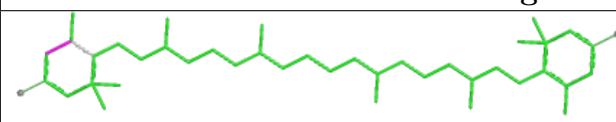
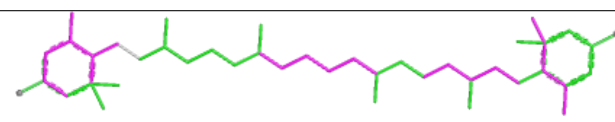
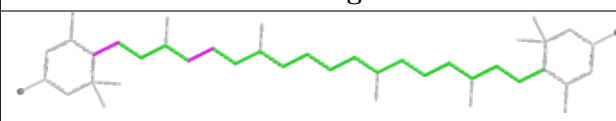
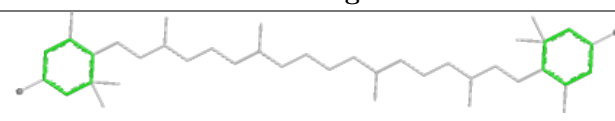
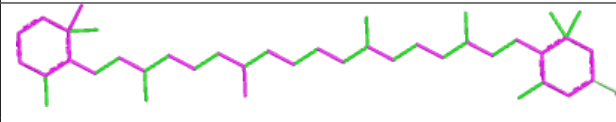
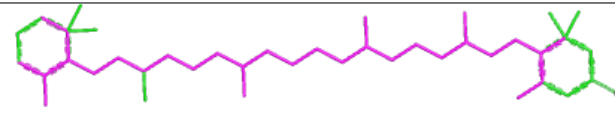
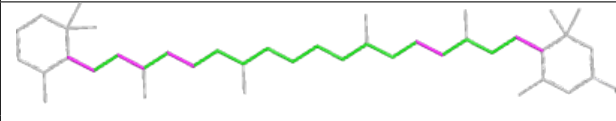
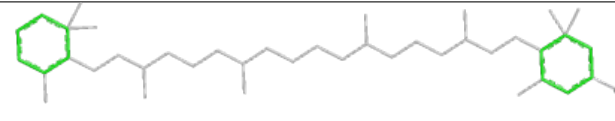
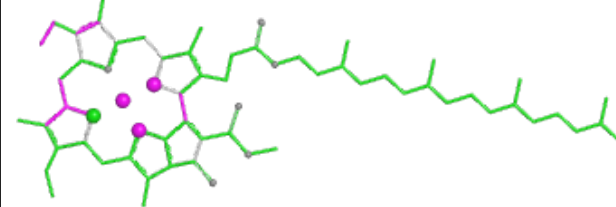
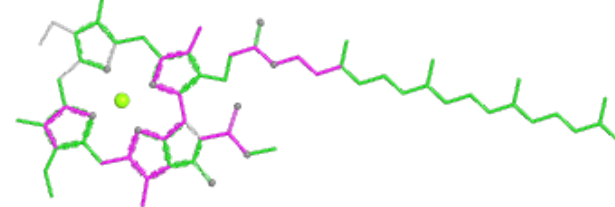
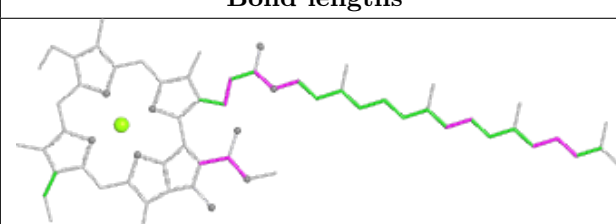
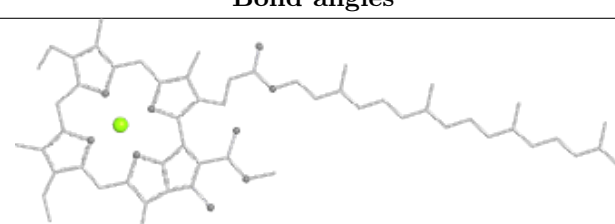
Ligand CLA b 614

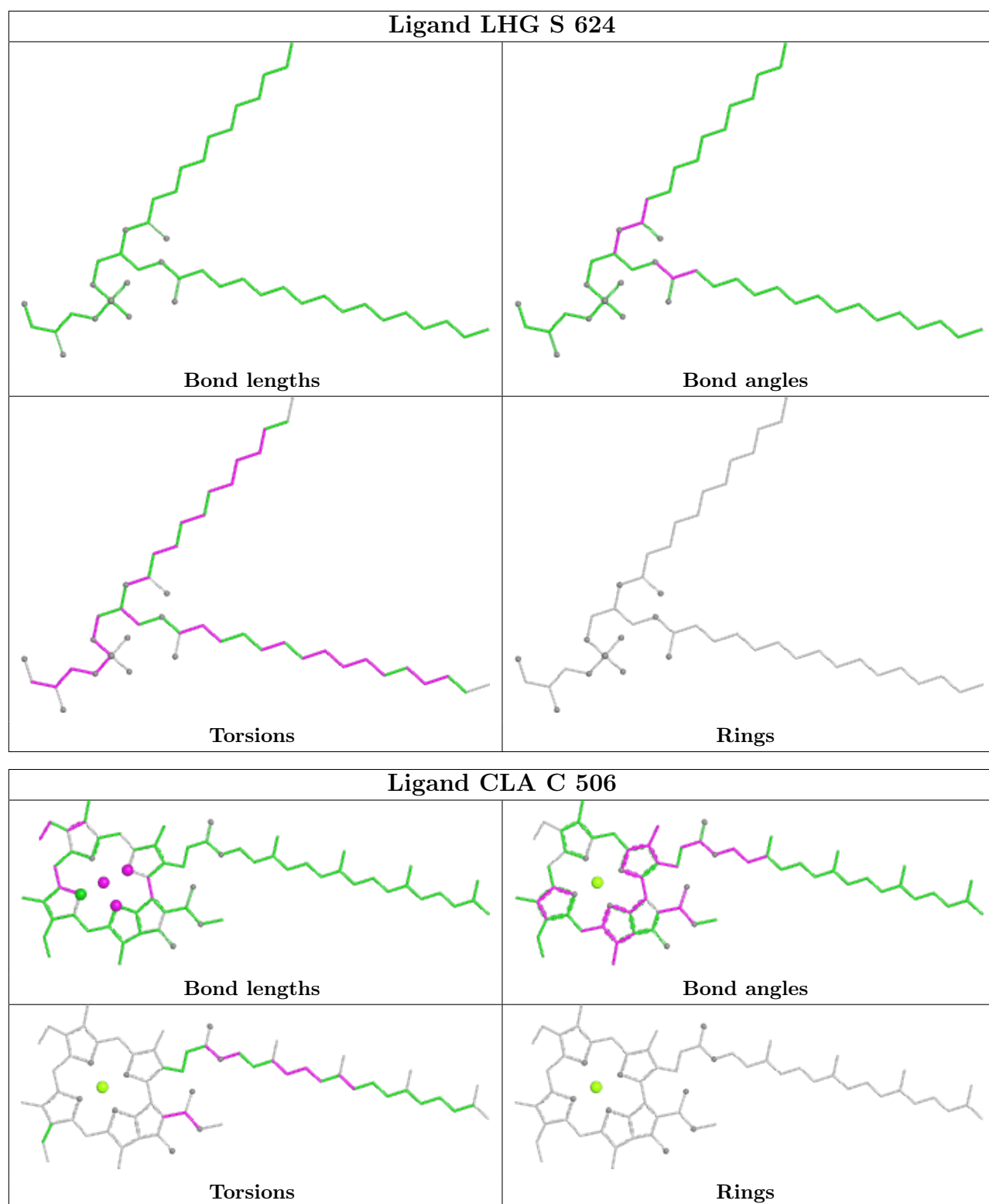


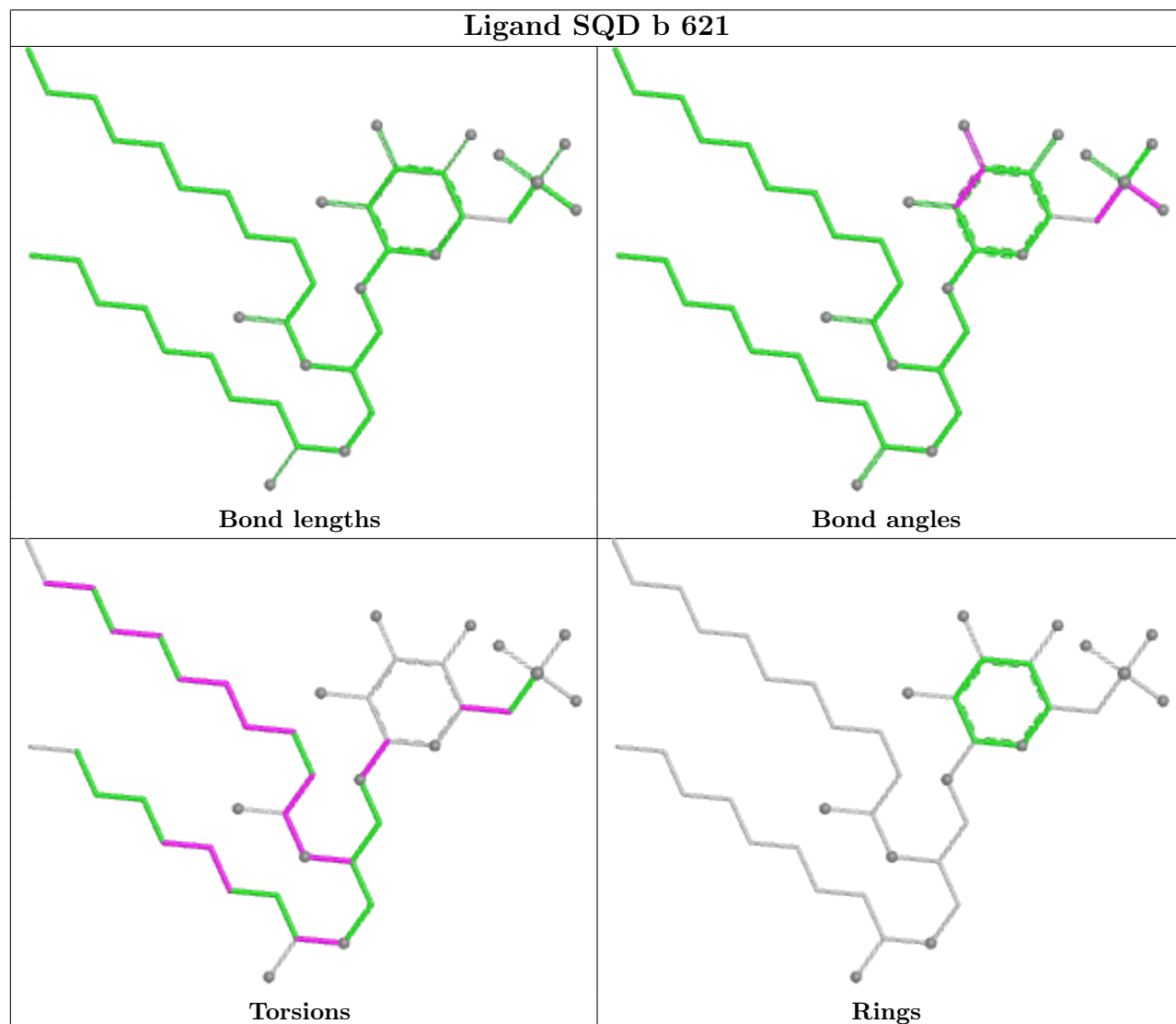
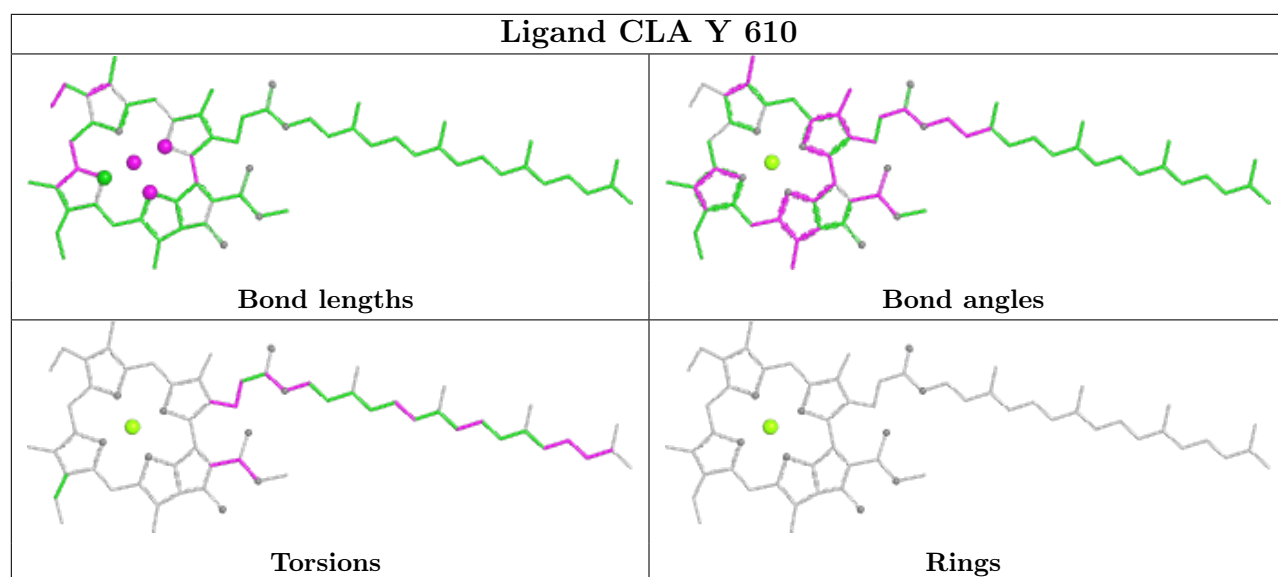
Ligand HEM F 101

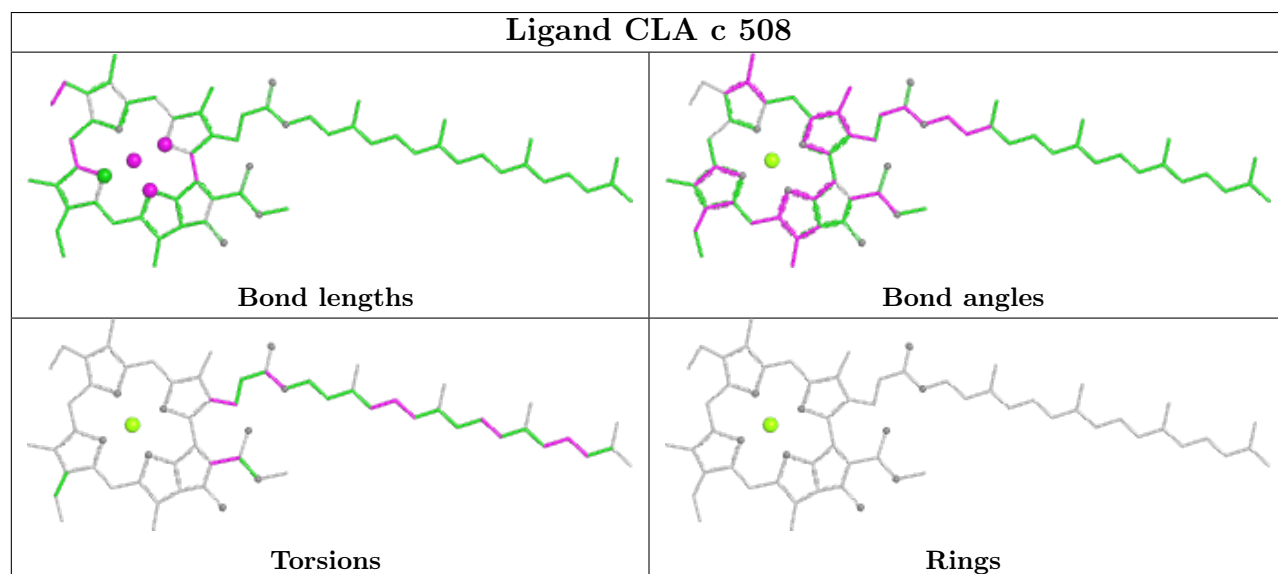
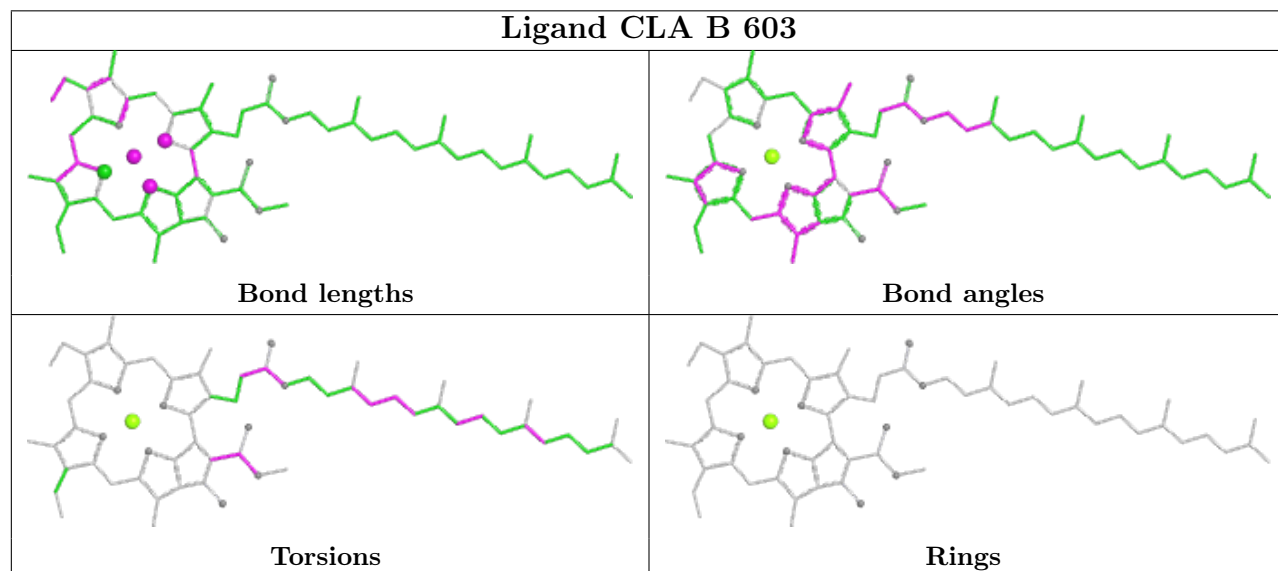
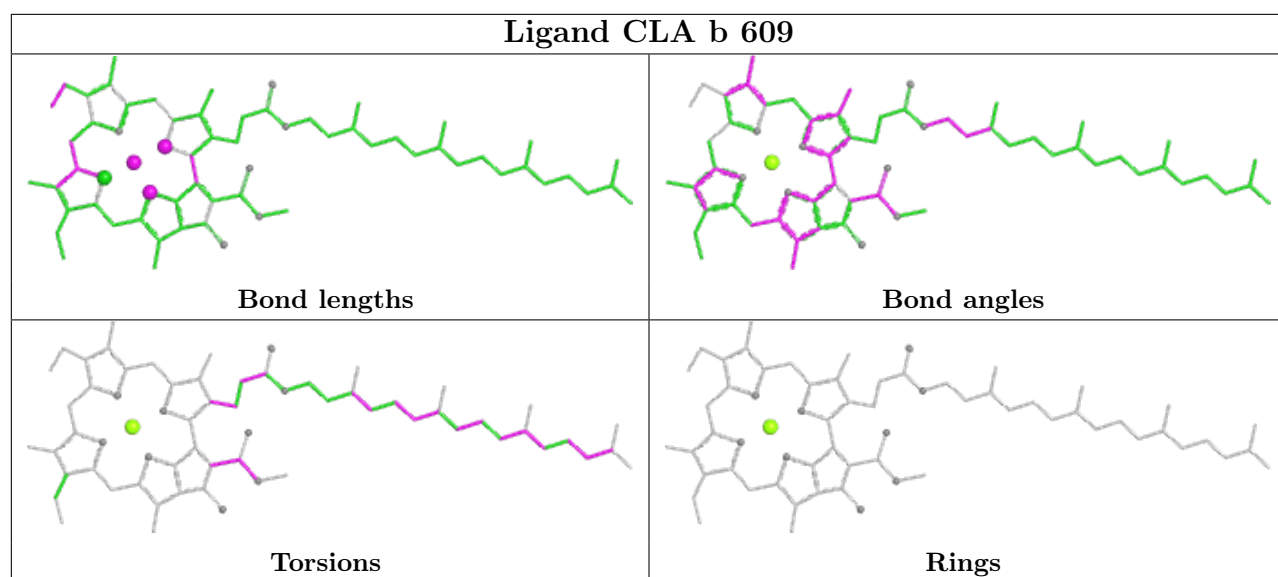


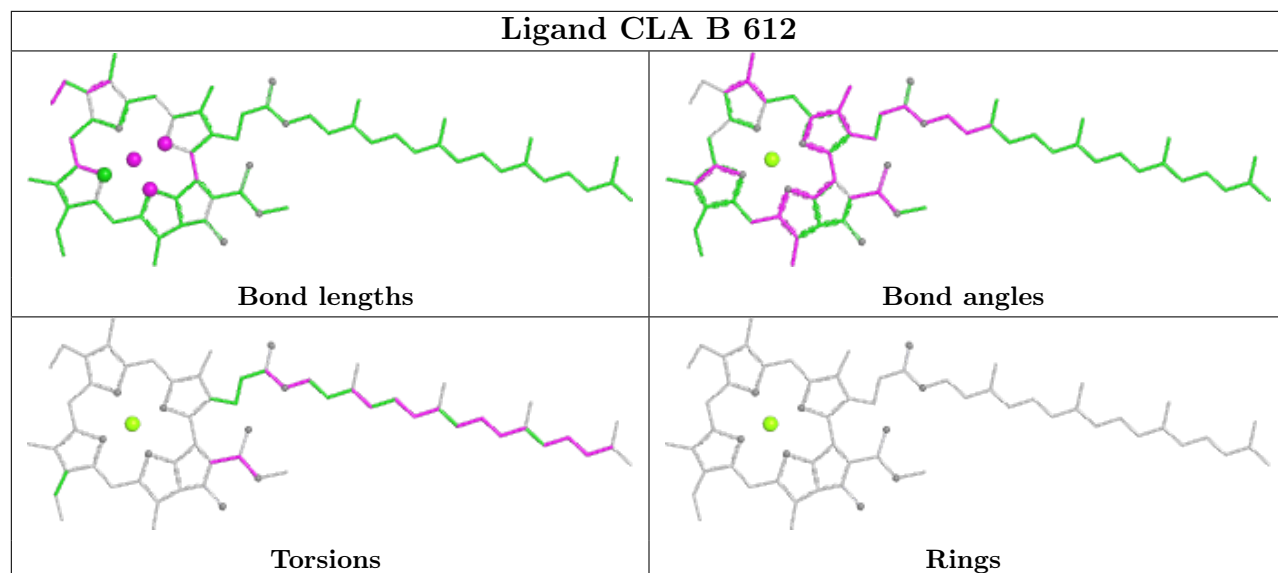
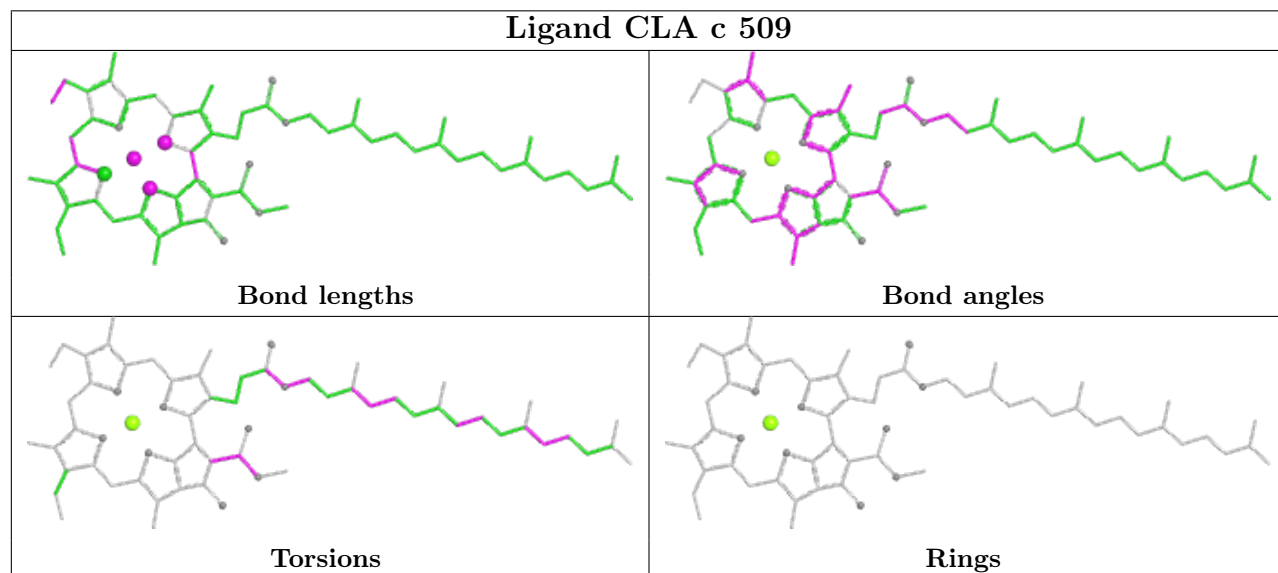
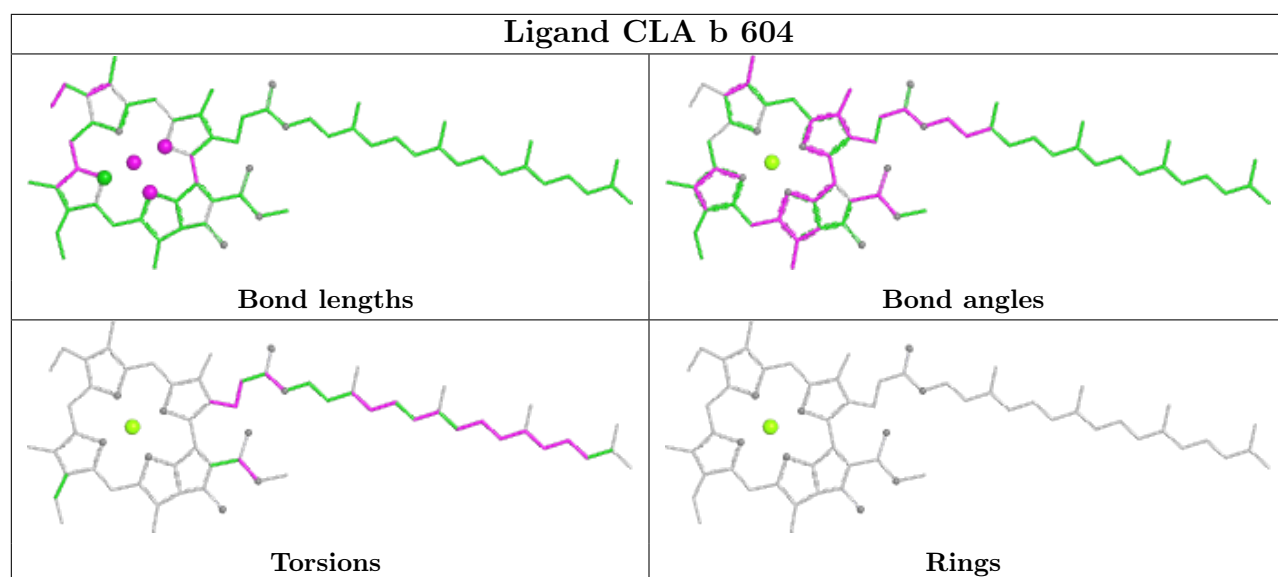


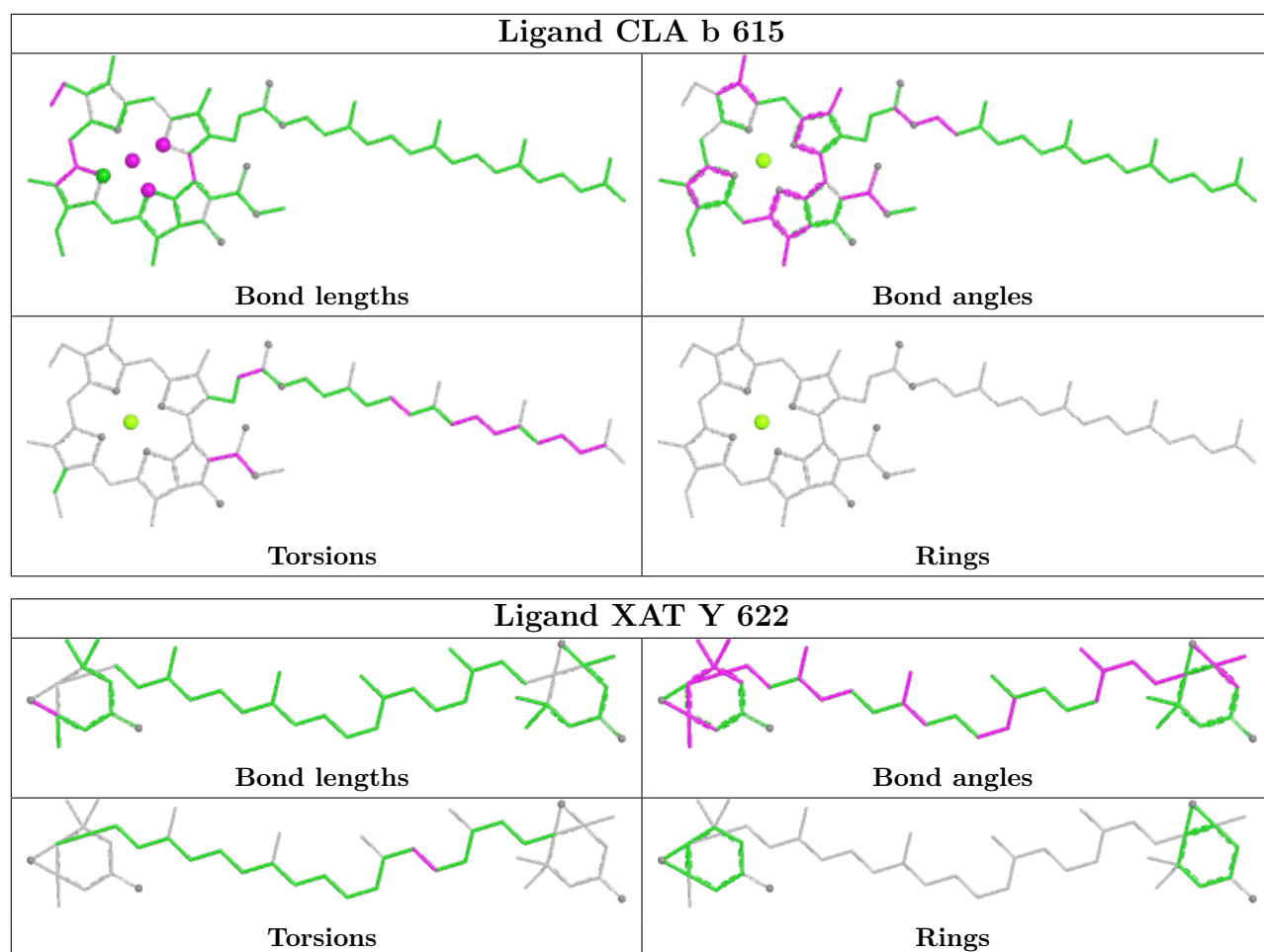
Ligand C7Z b 620	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT N 621	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand RRX H 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA B 611	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

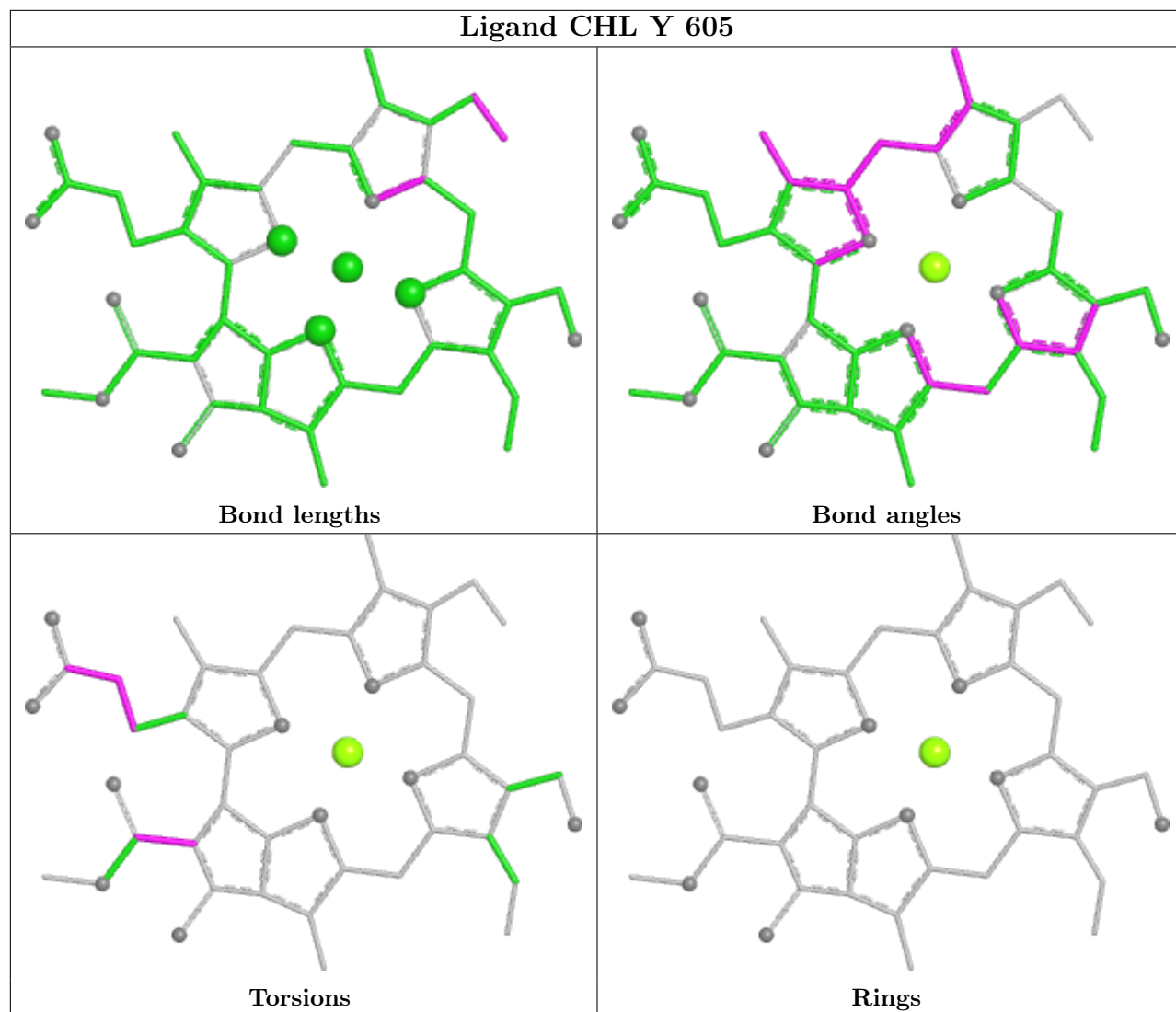




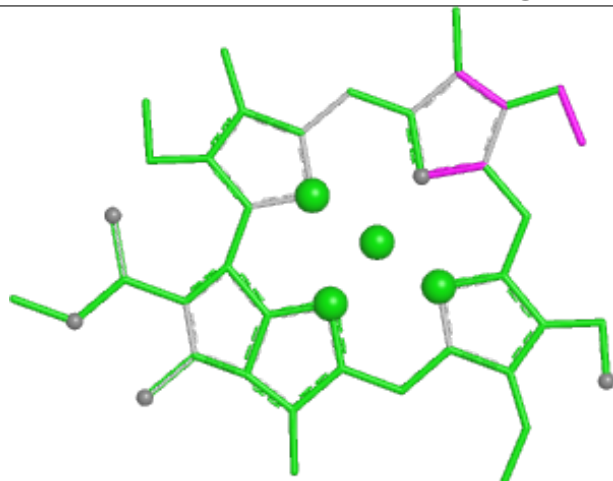




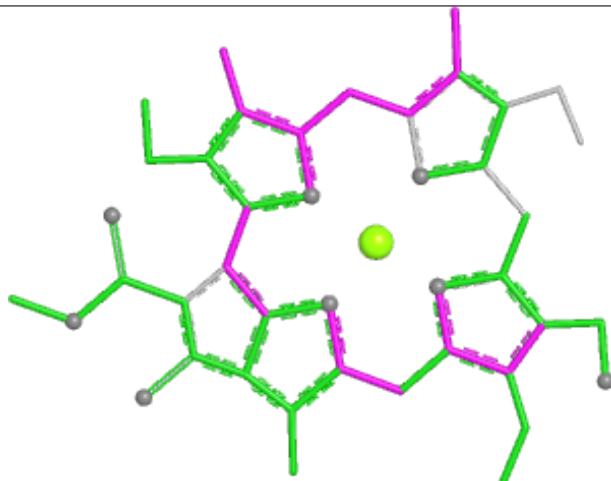




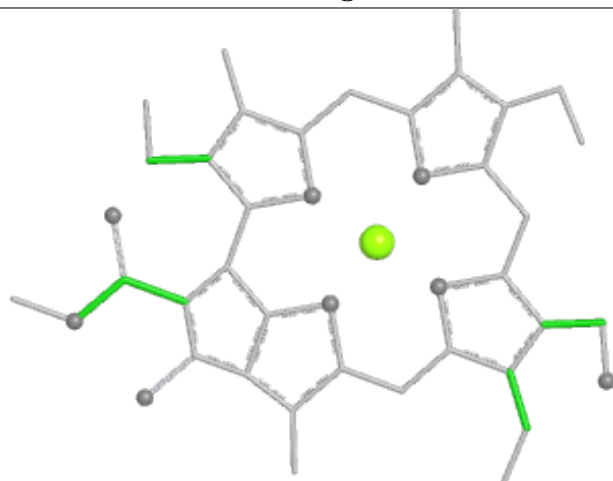
Ligand CHL S 607



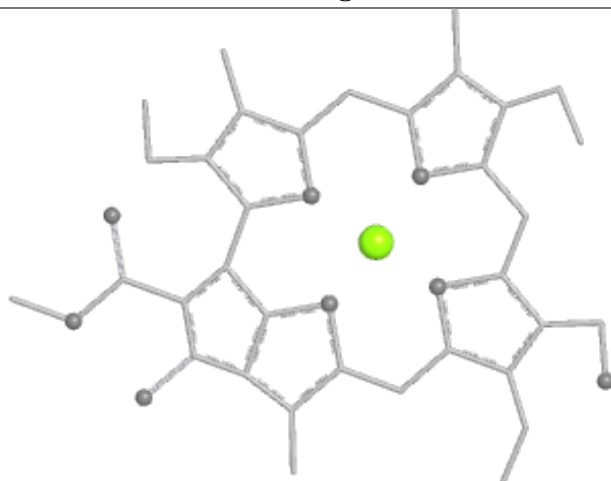
Bond lengths



Bond angles

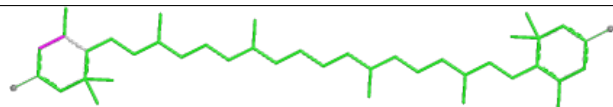


Torsions

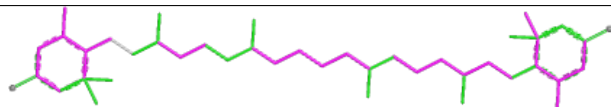


Rings

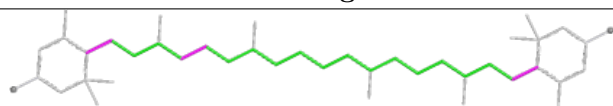
Ligand LUT Y 621



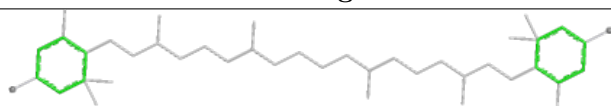
Bond lengths



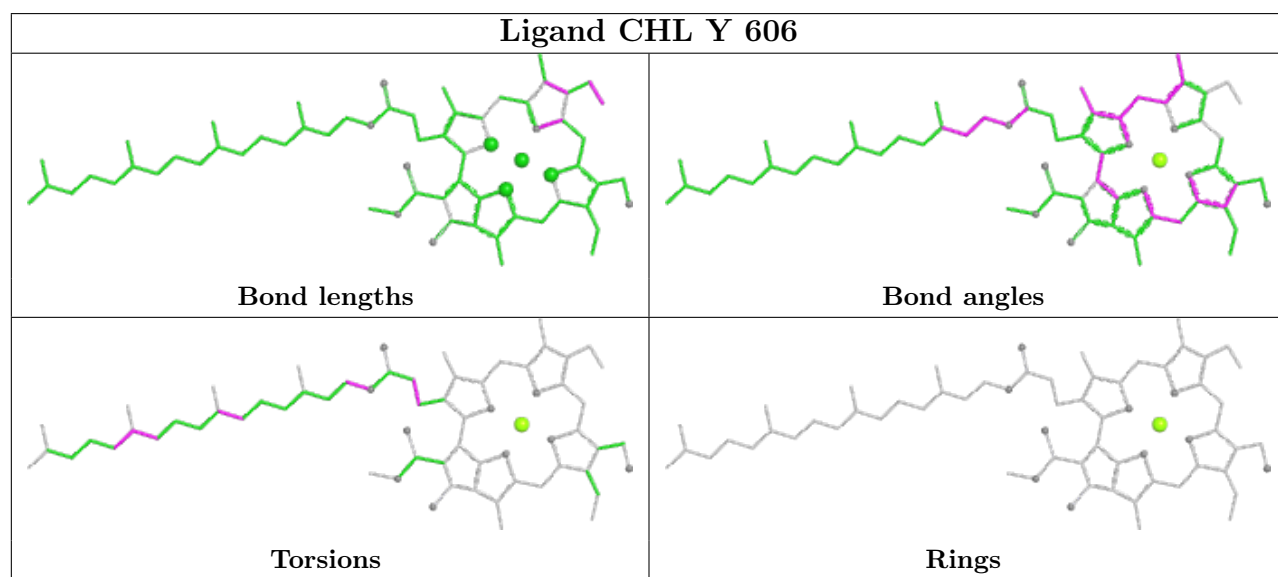
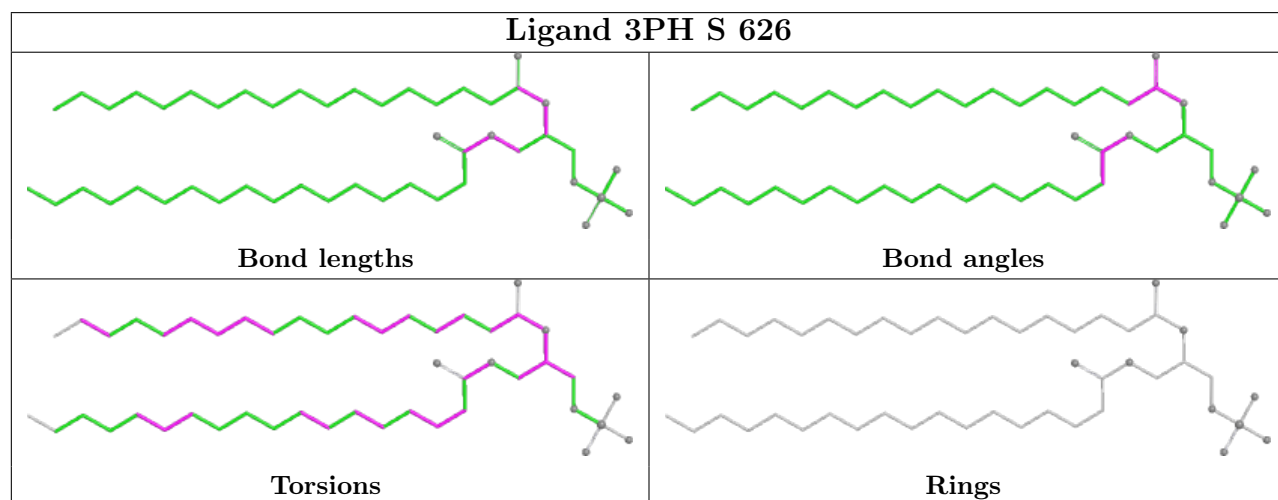
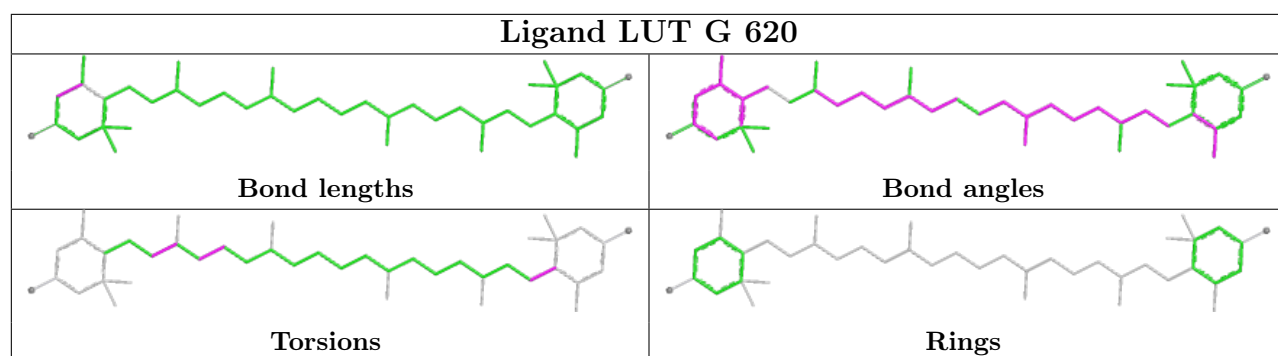
Bond angles

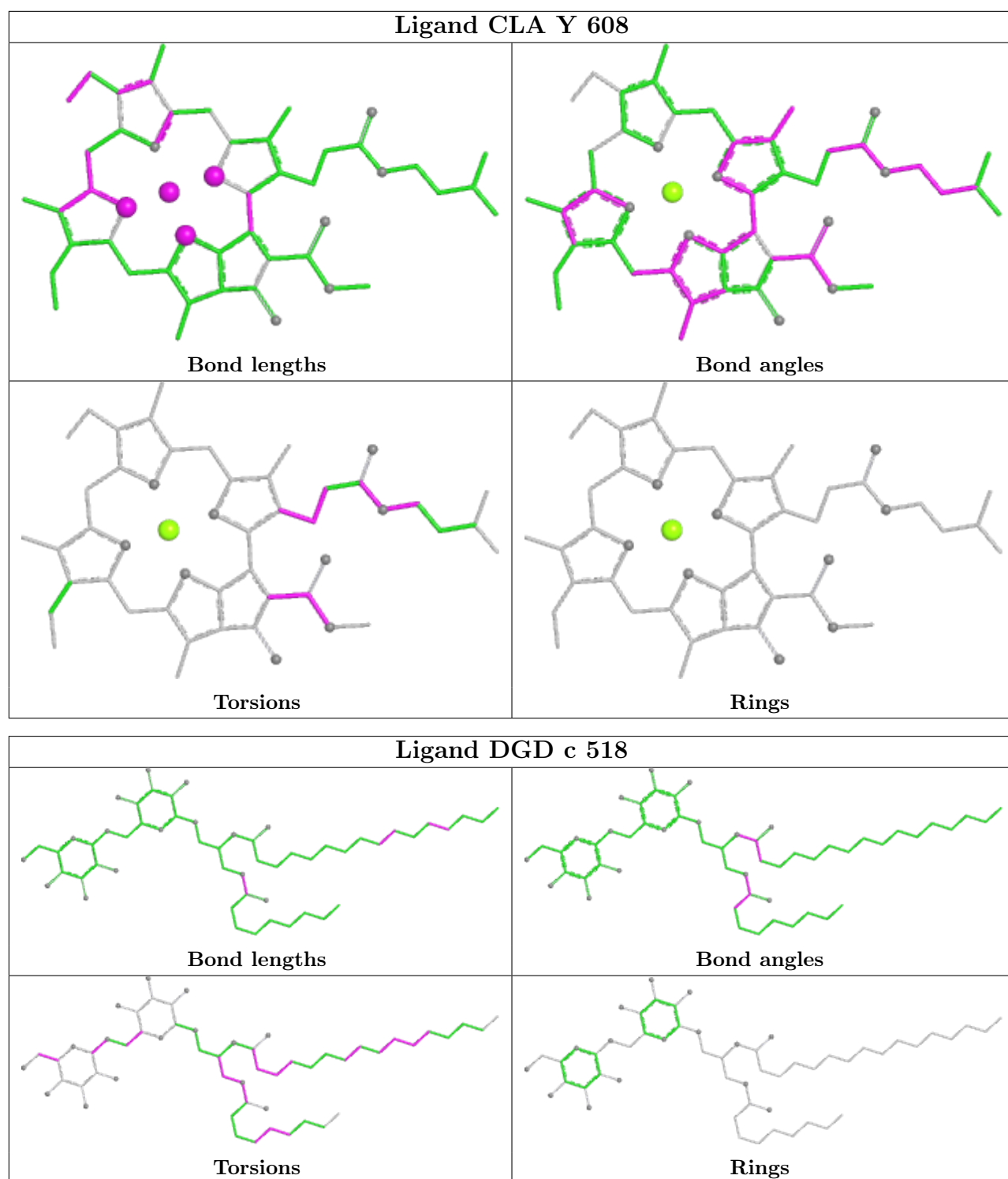


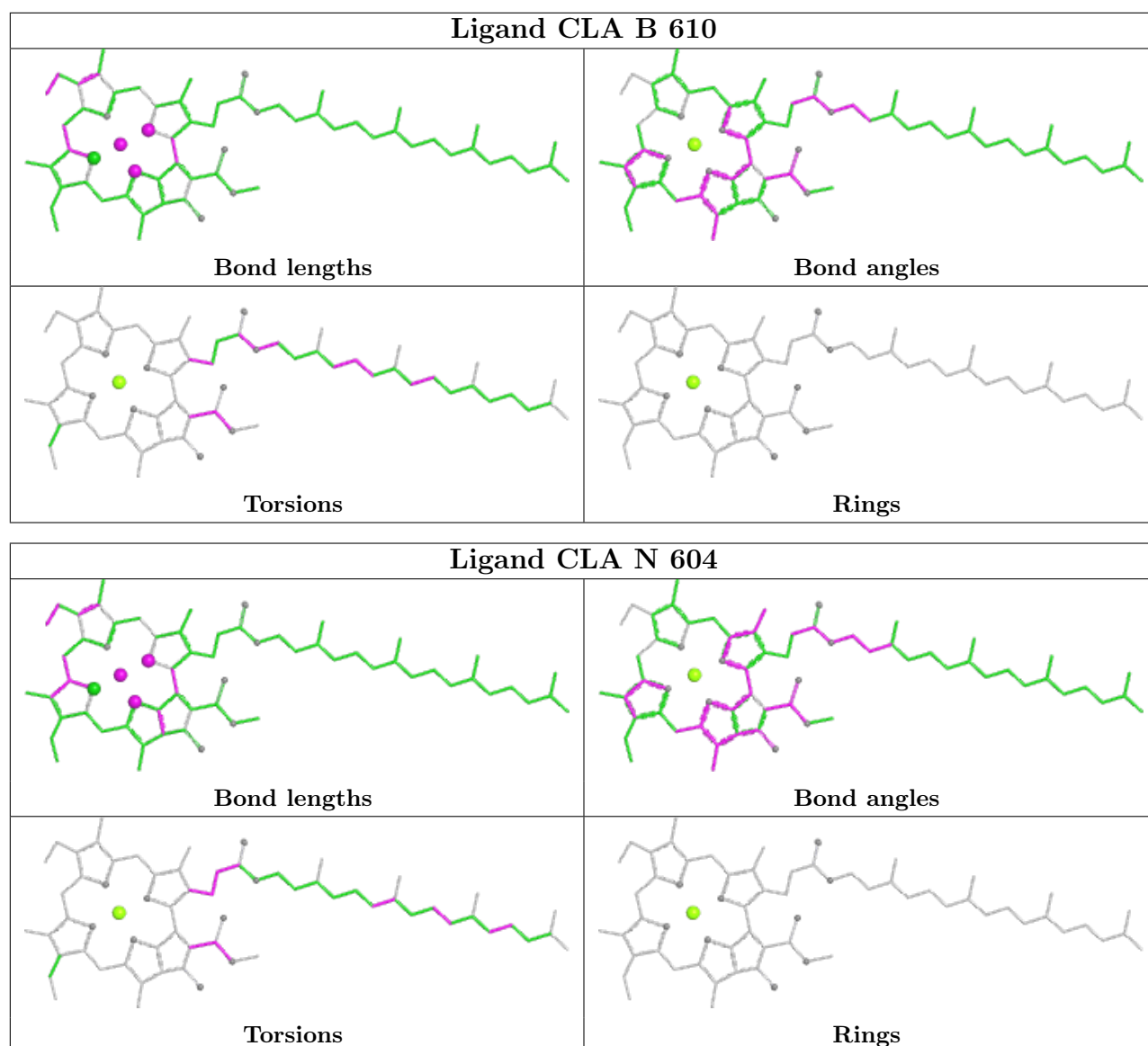
Torsions

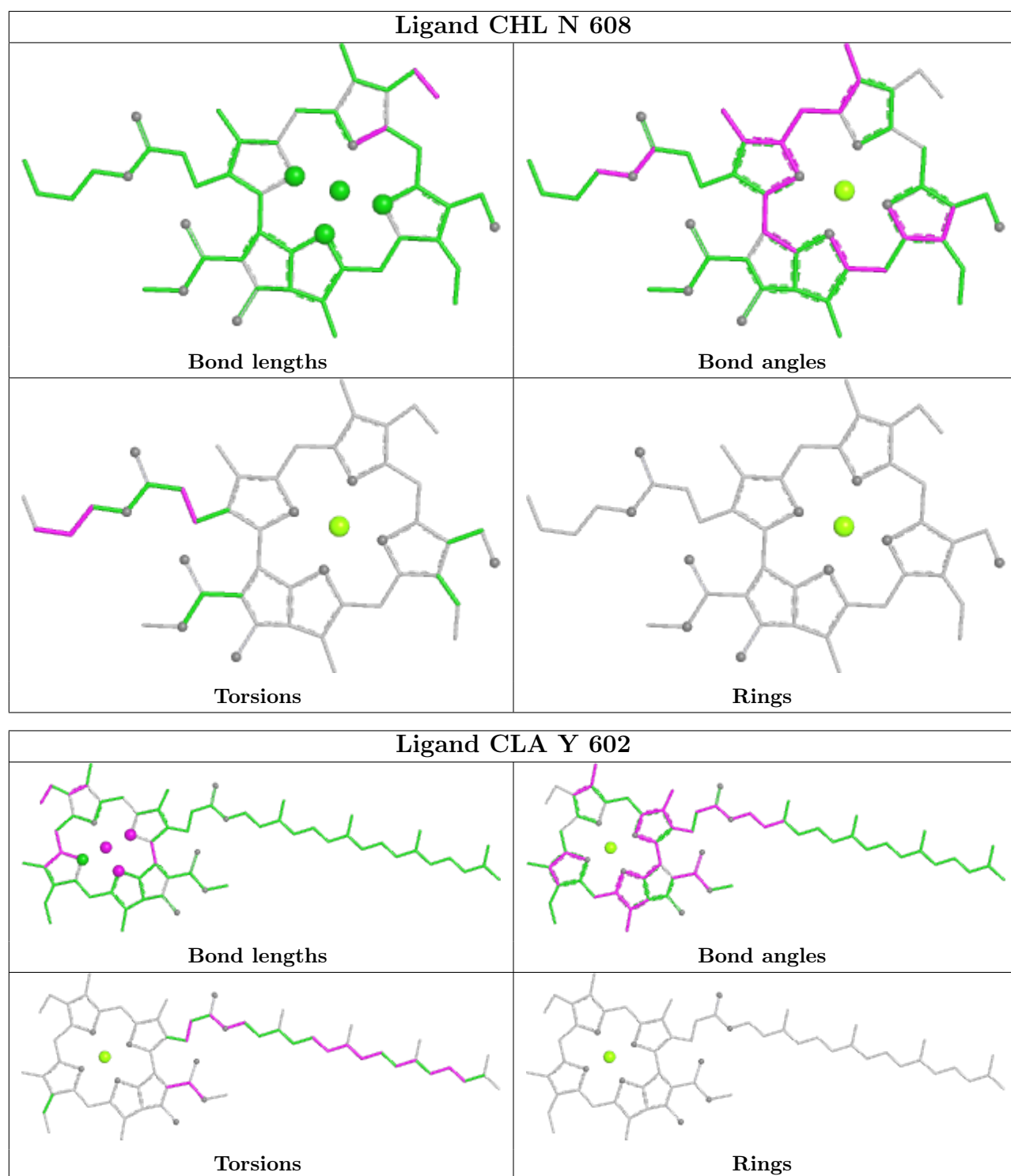


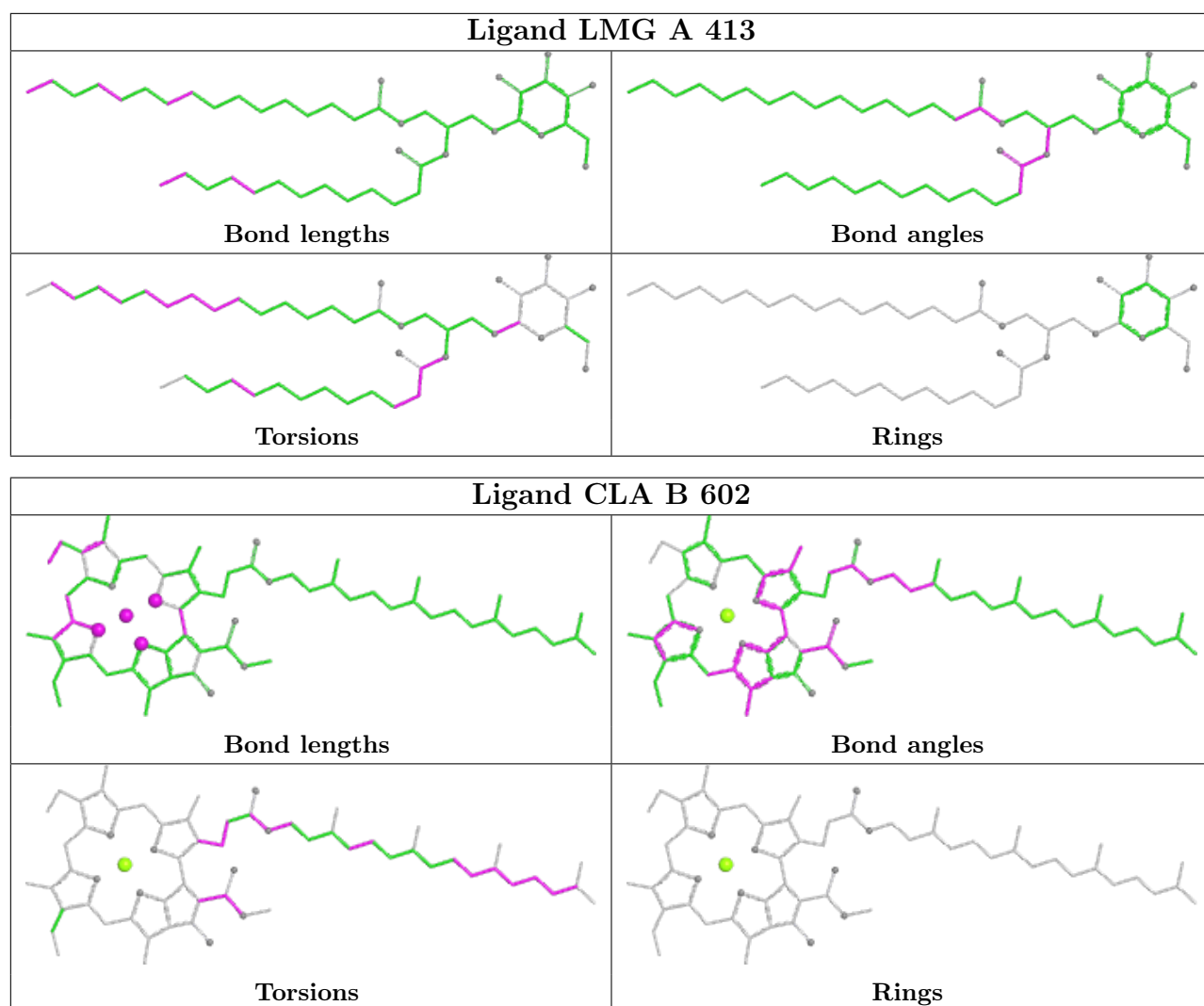
Rings

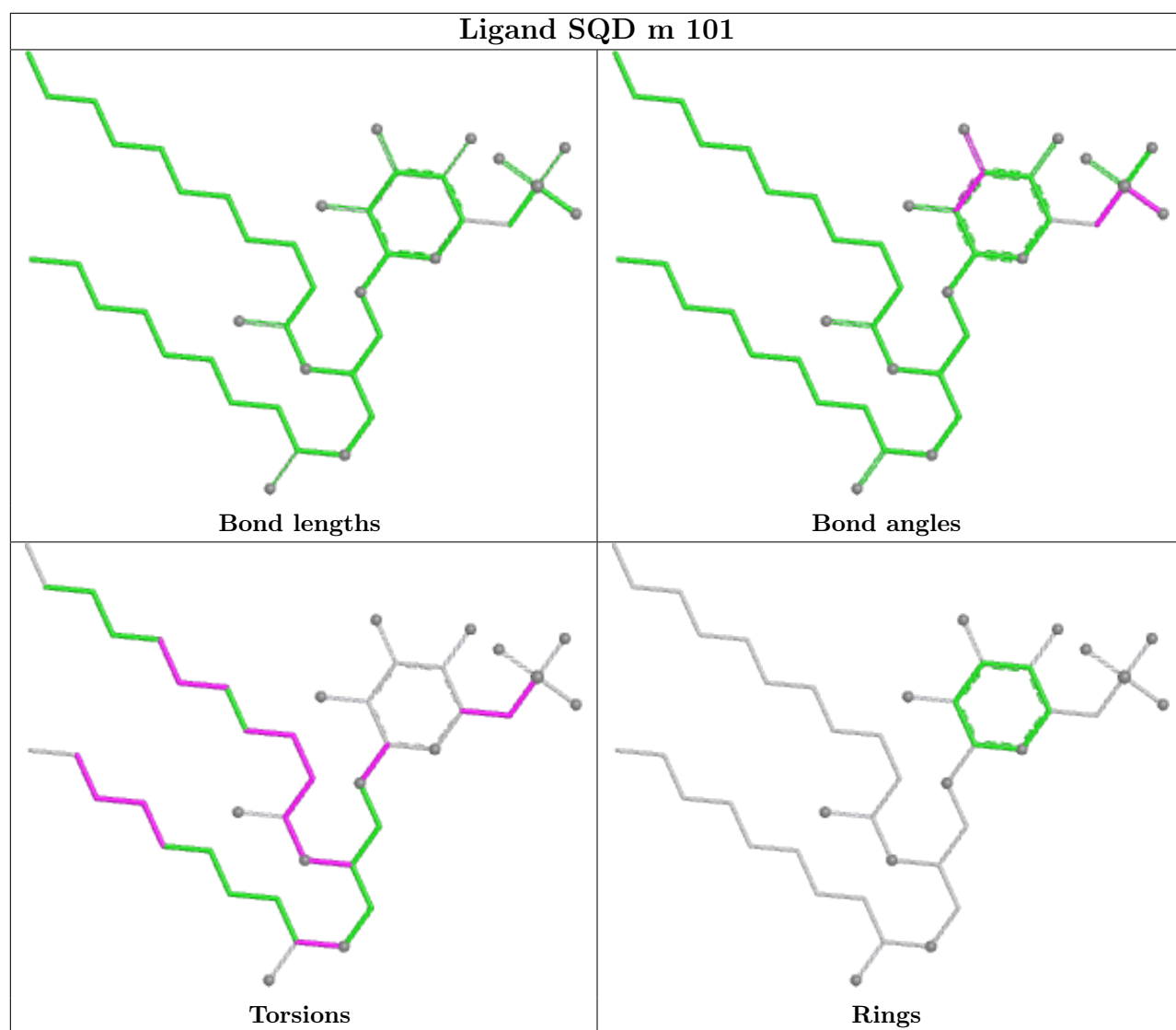


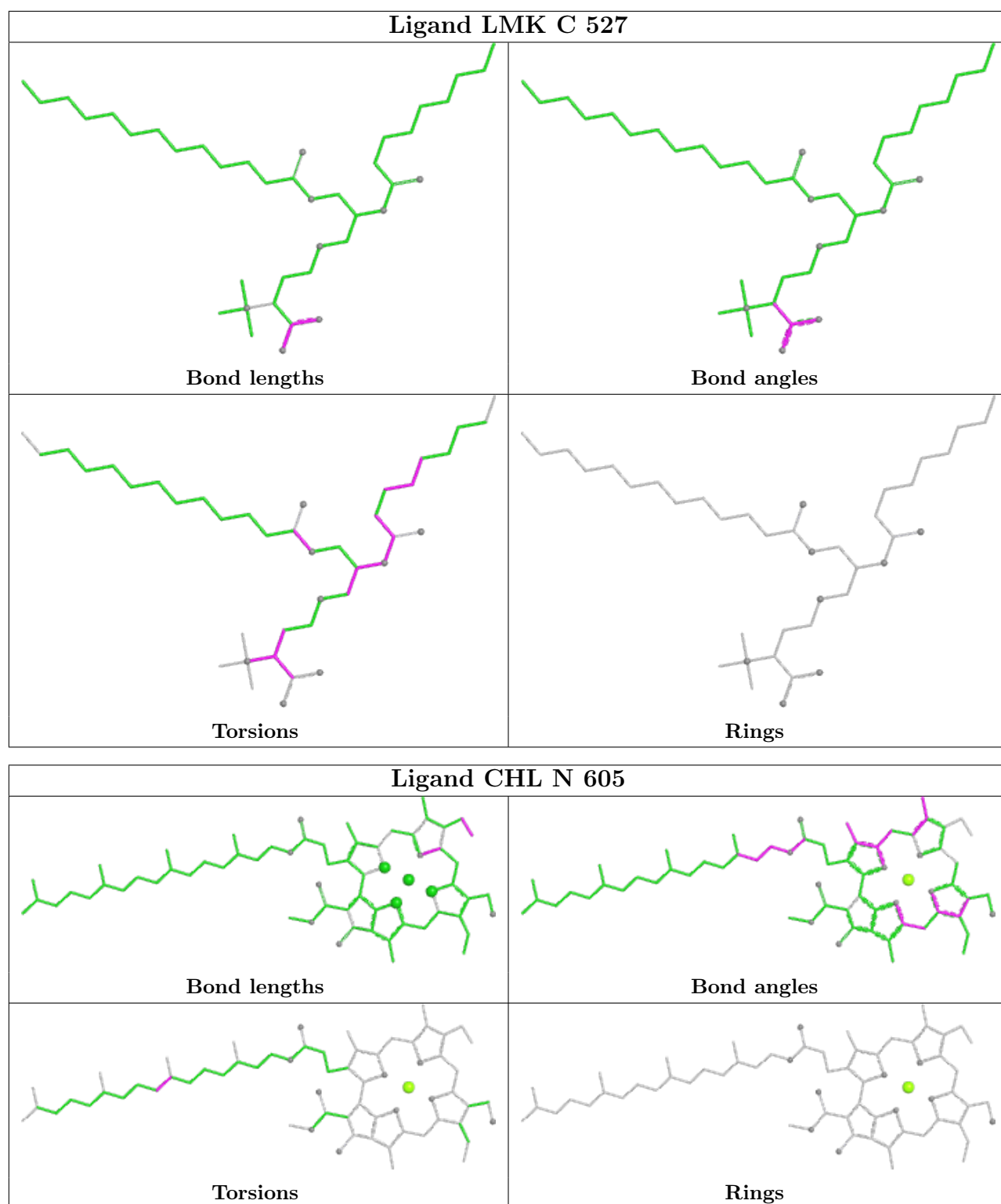


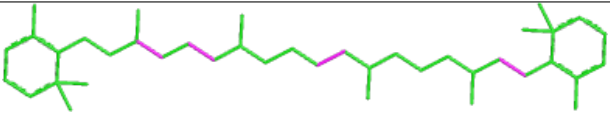
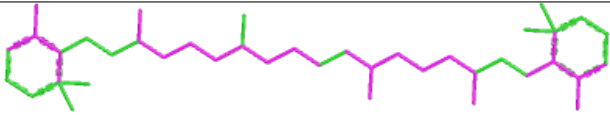
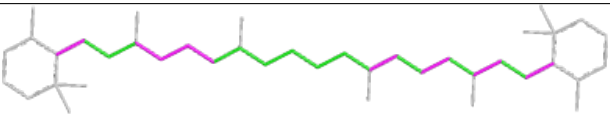
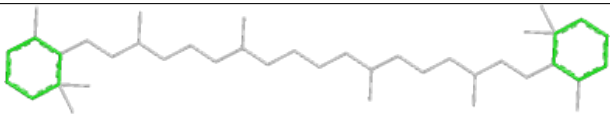
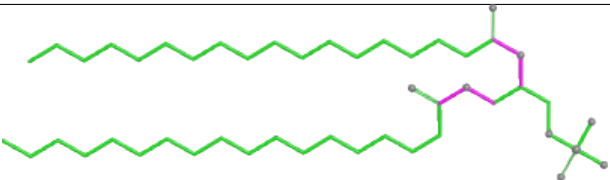
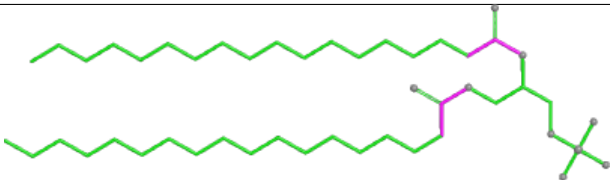
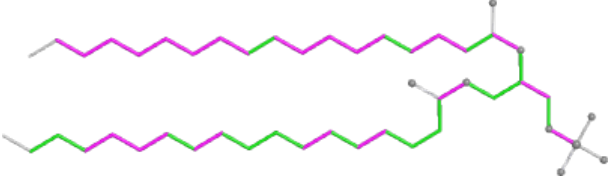
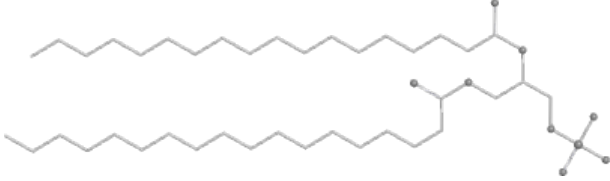
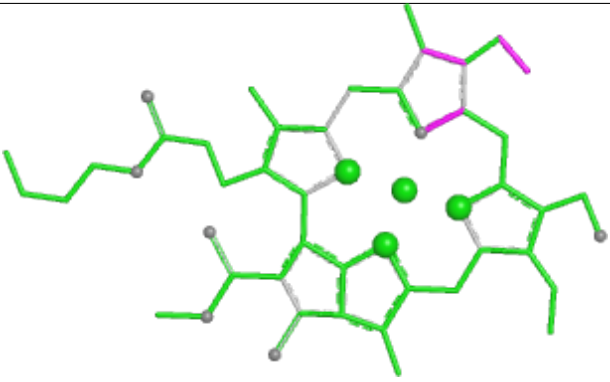
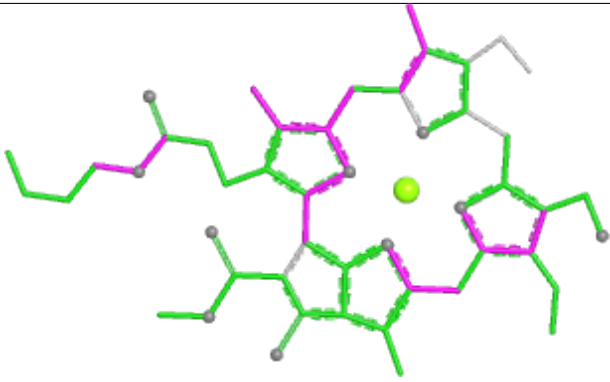
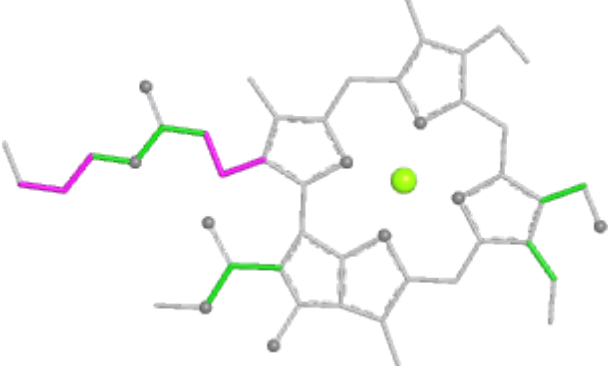
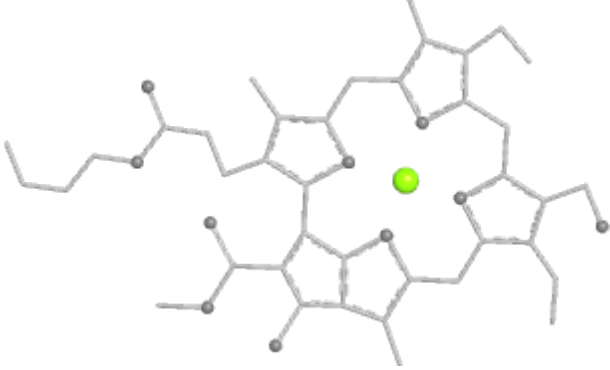


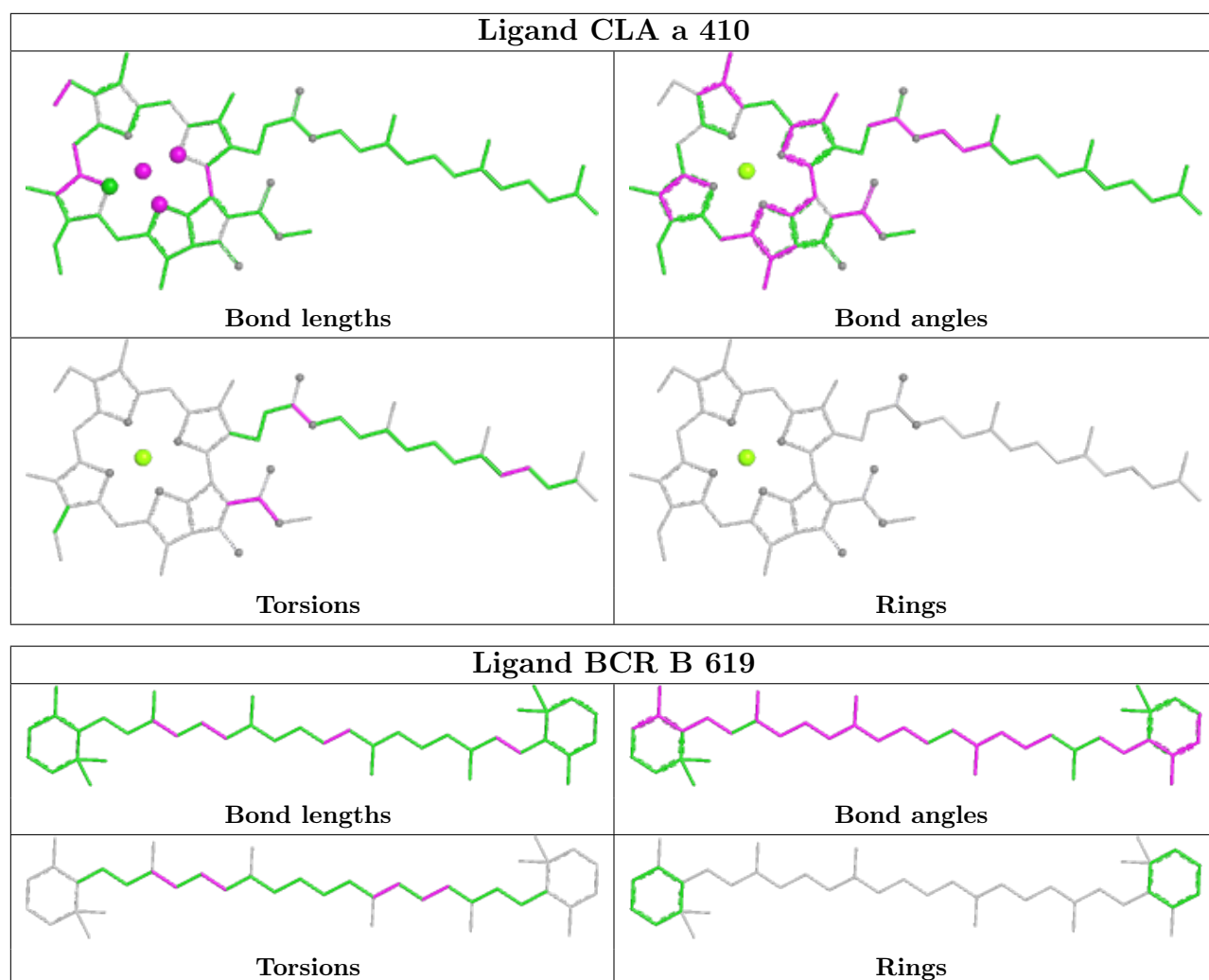


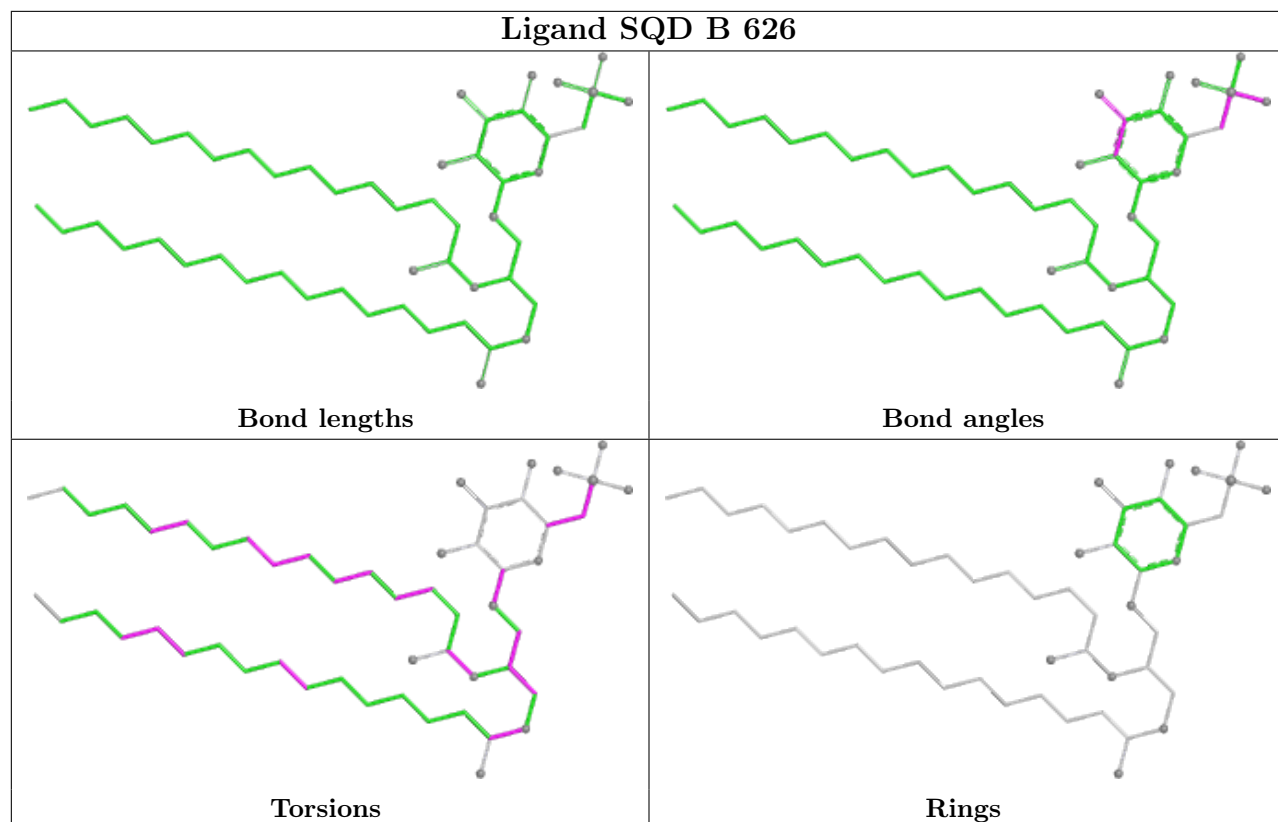


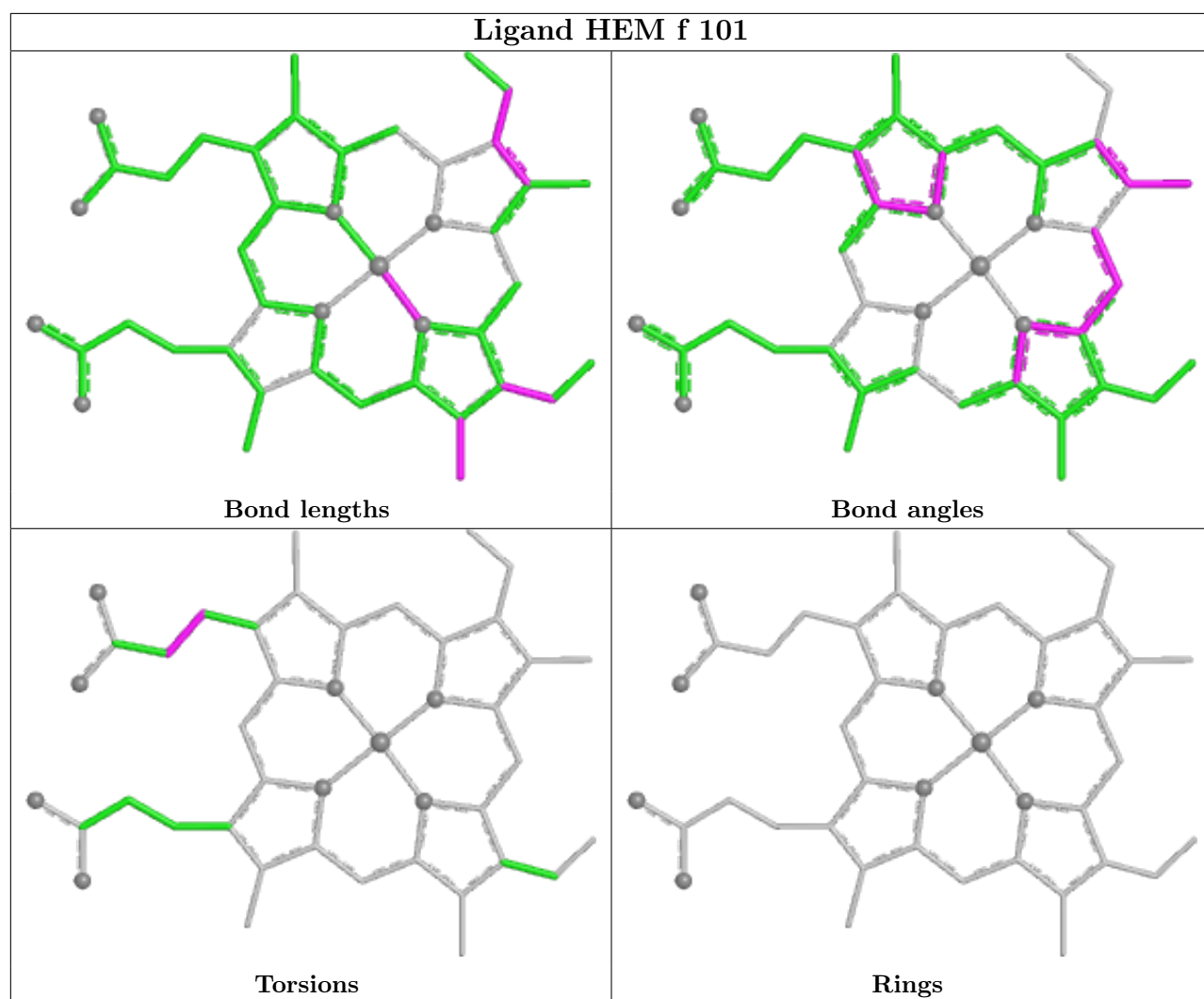




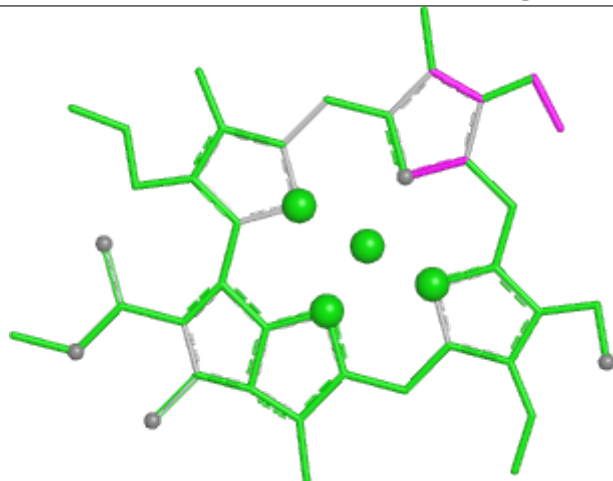
Ligand BCR d 404	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand 3PH B 624	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CHL G 606	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



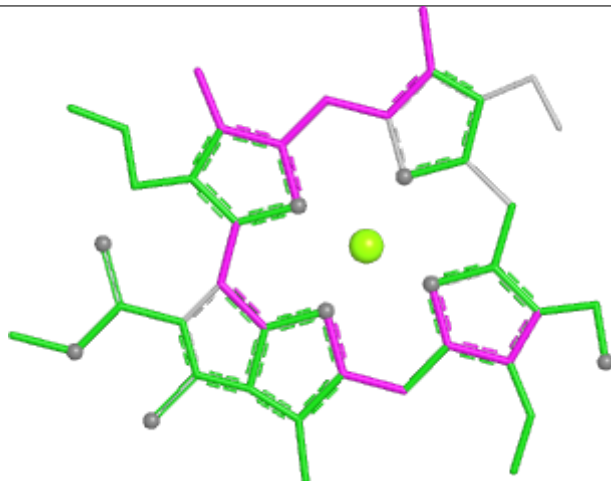




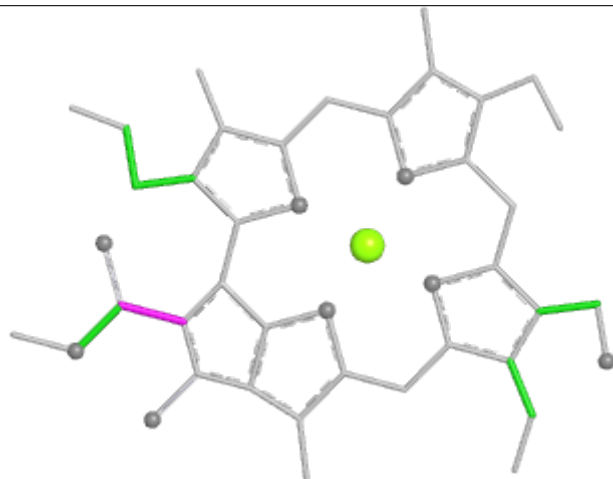
Ligand CHL S 606



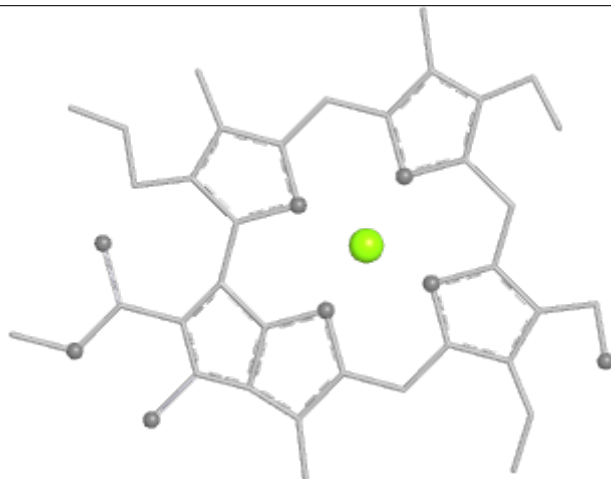
Bond lengths



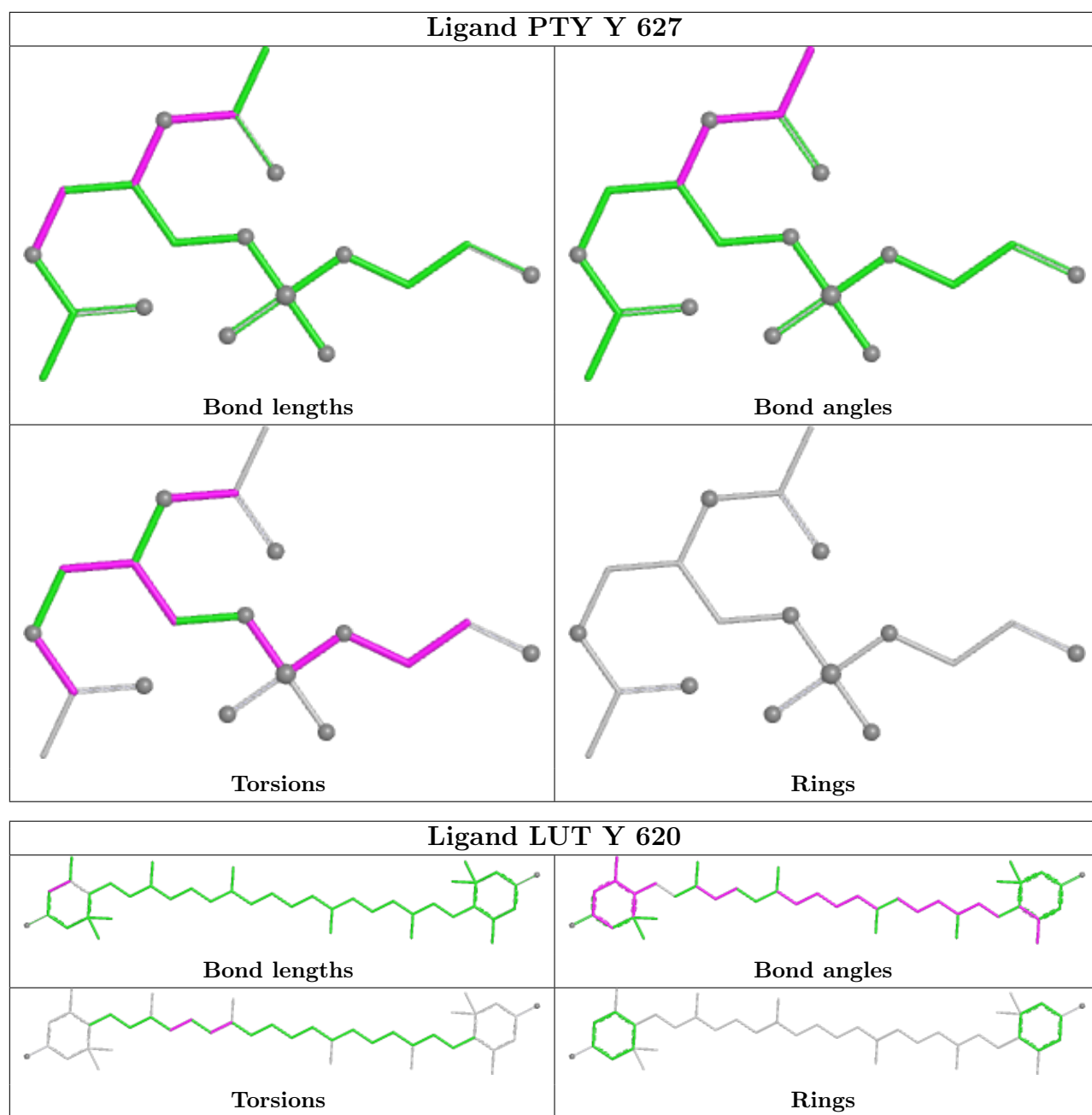
Bond angles

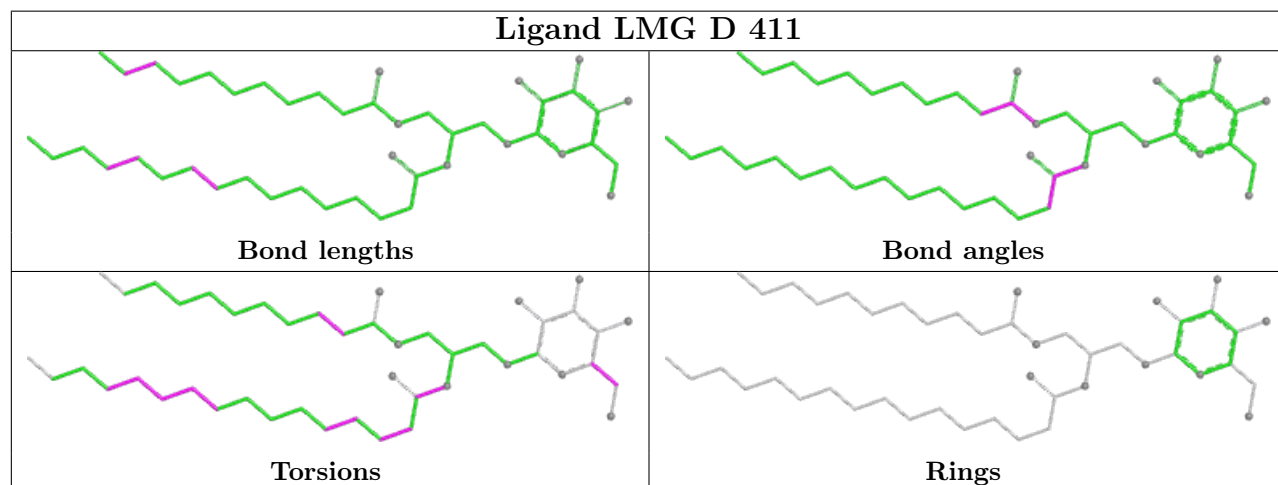
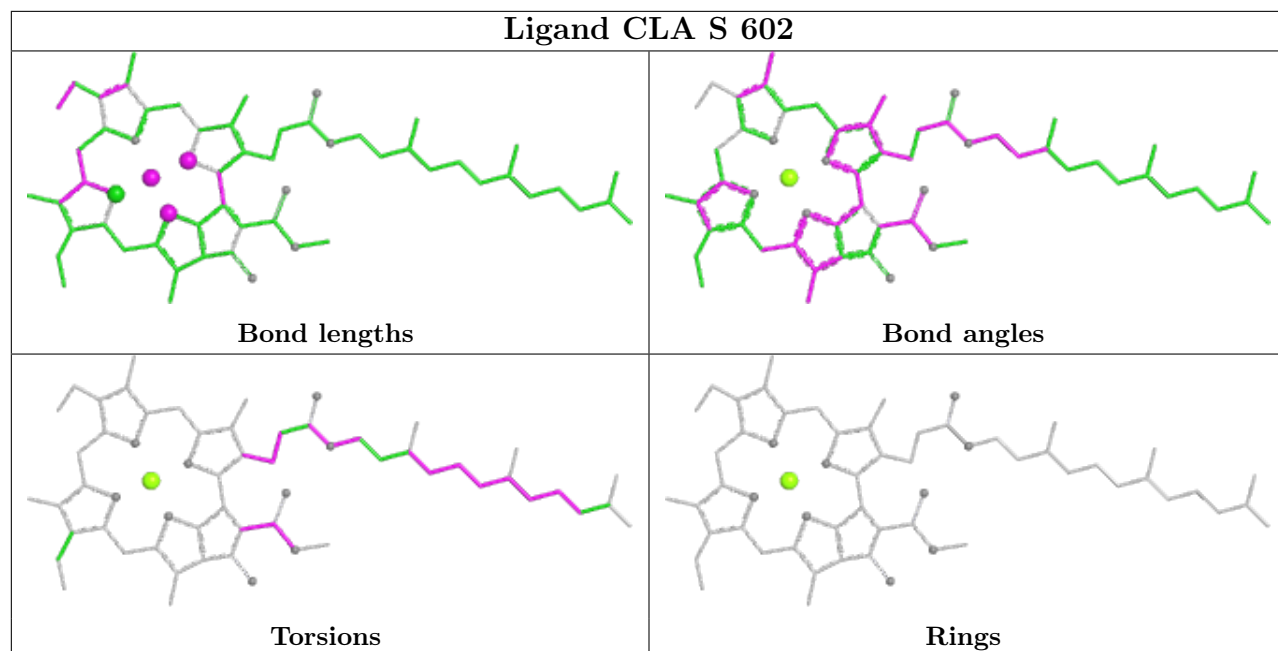


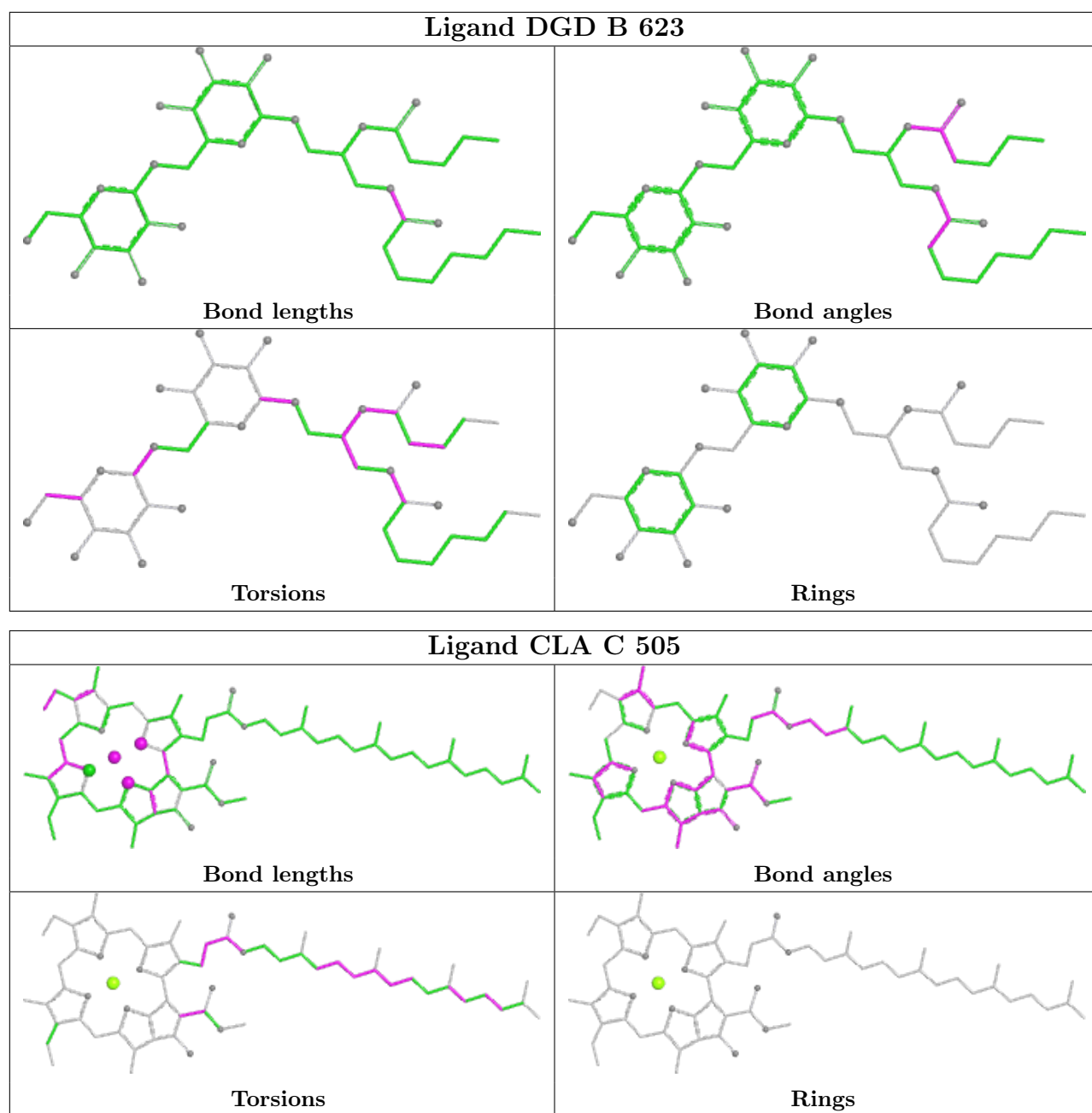
Torsions

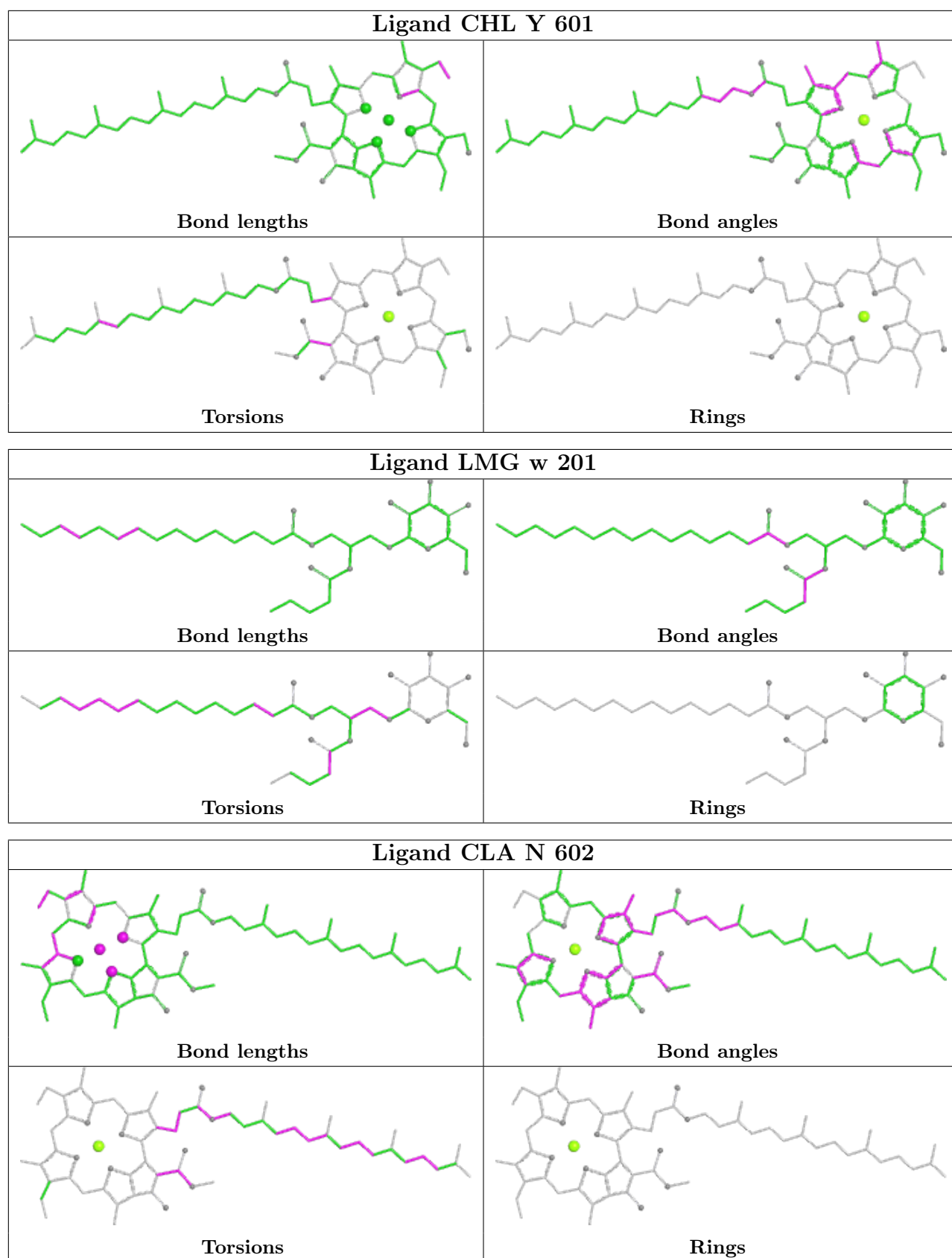


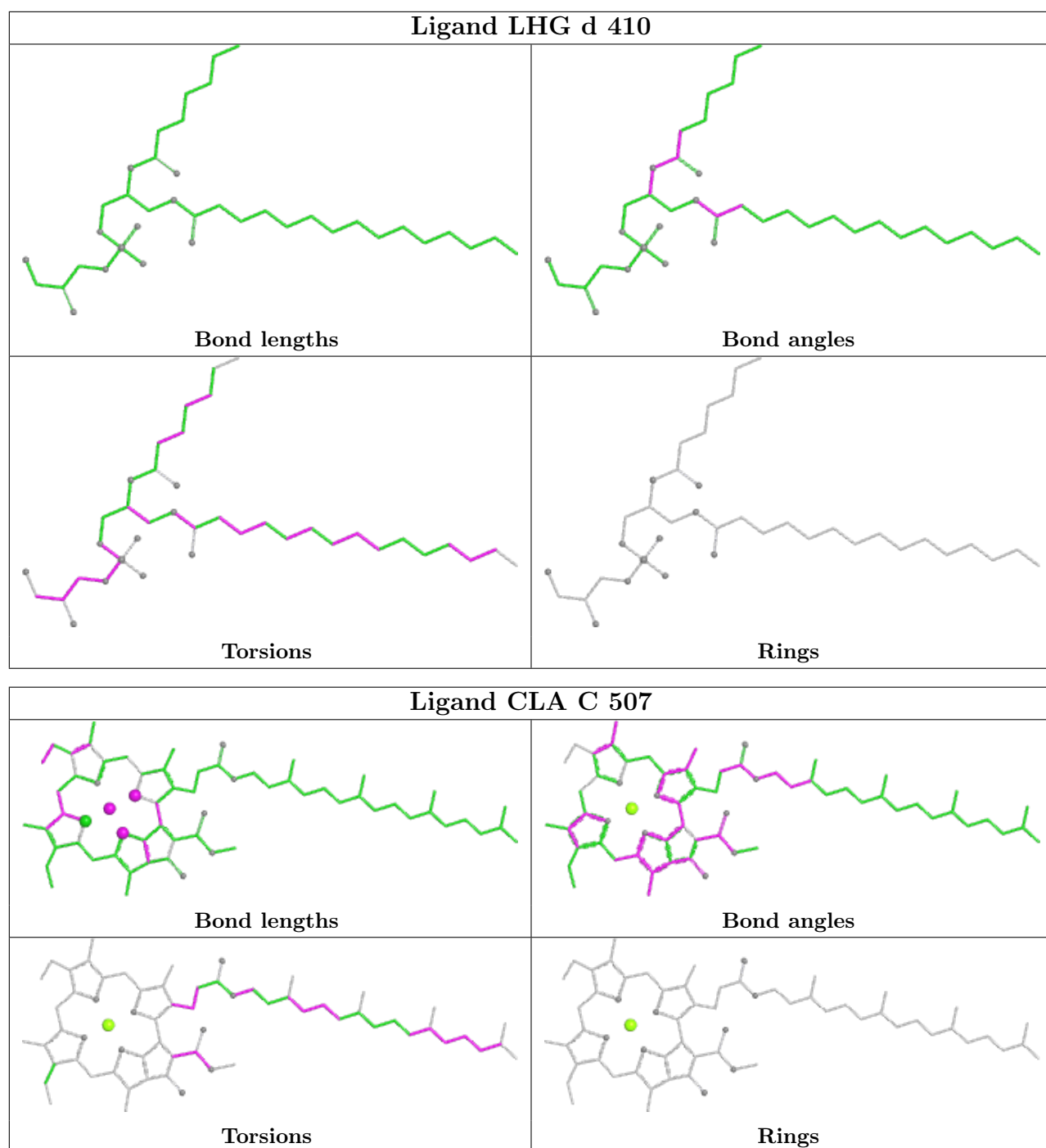
Rings

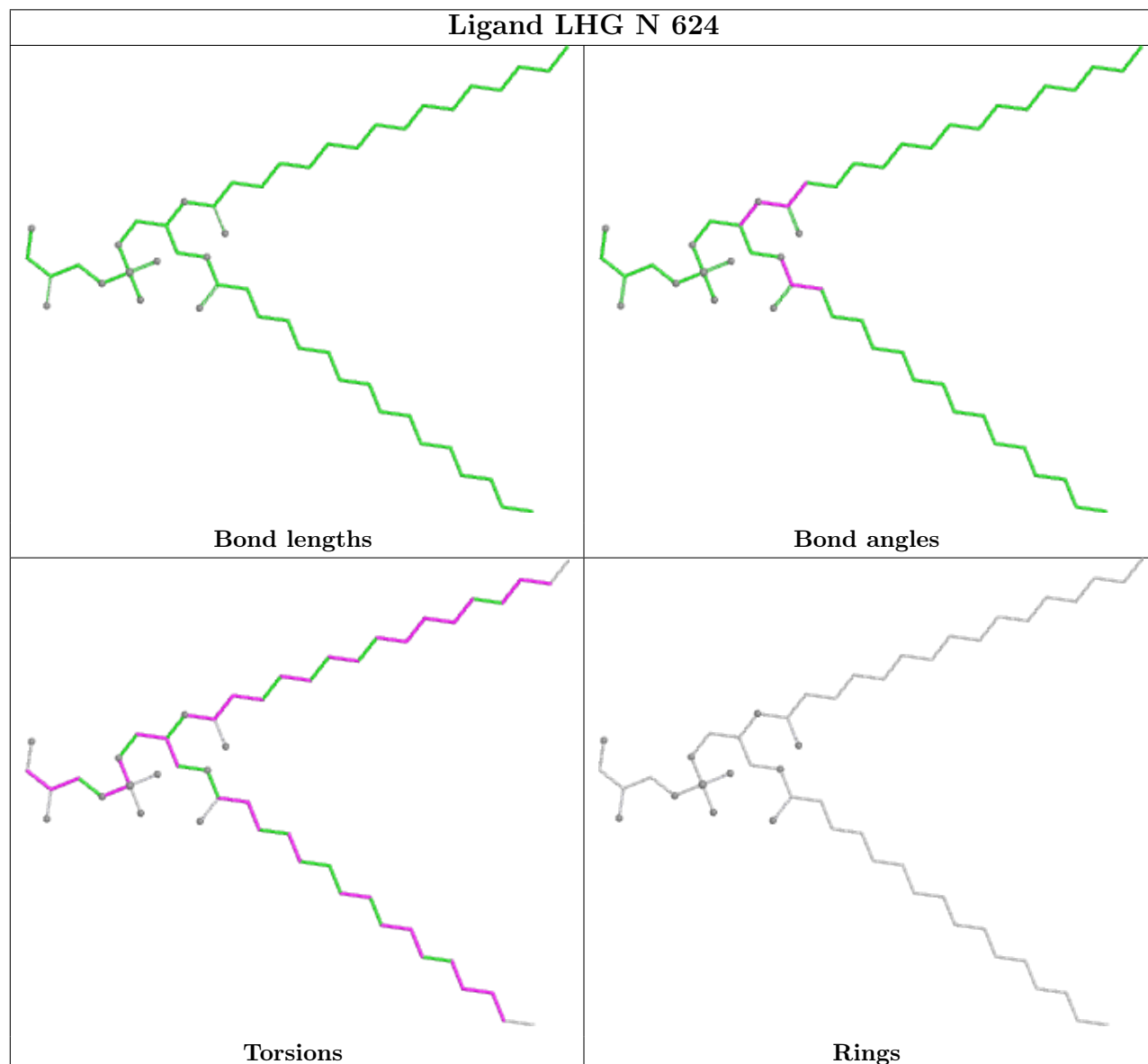
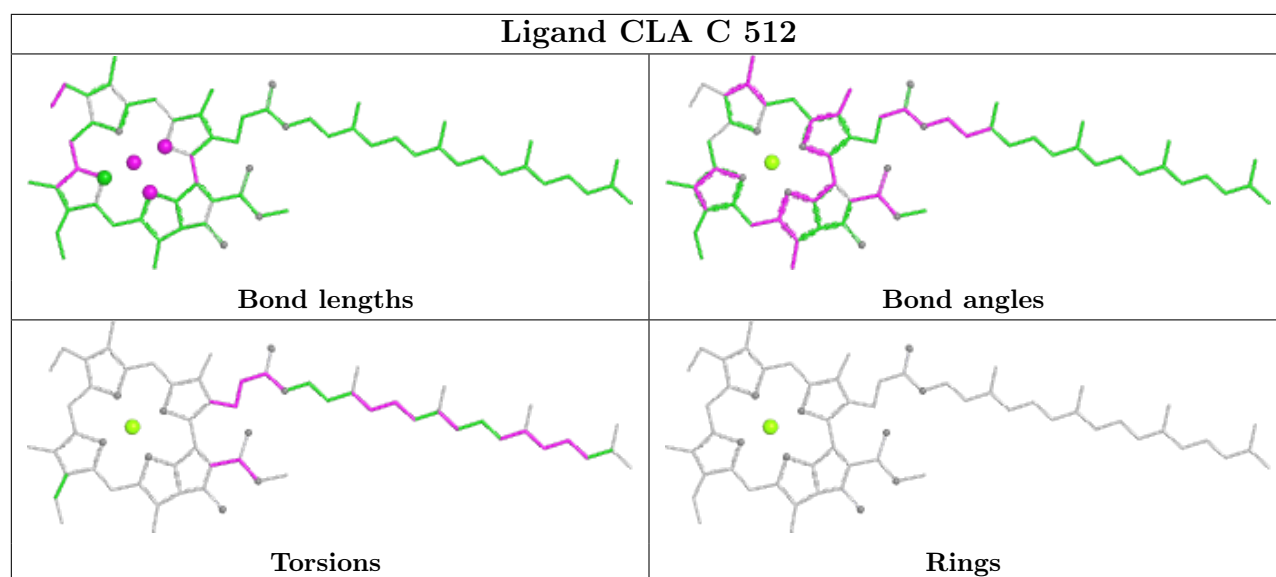


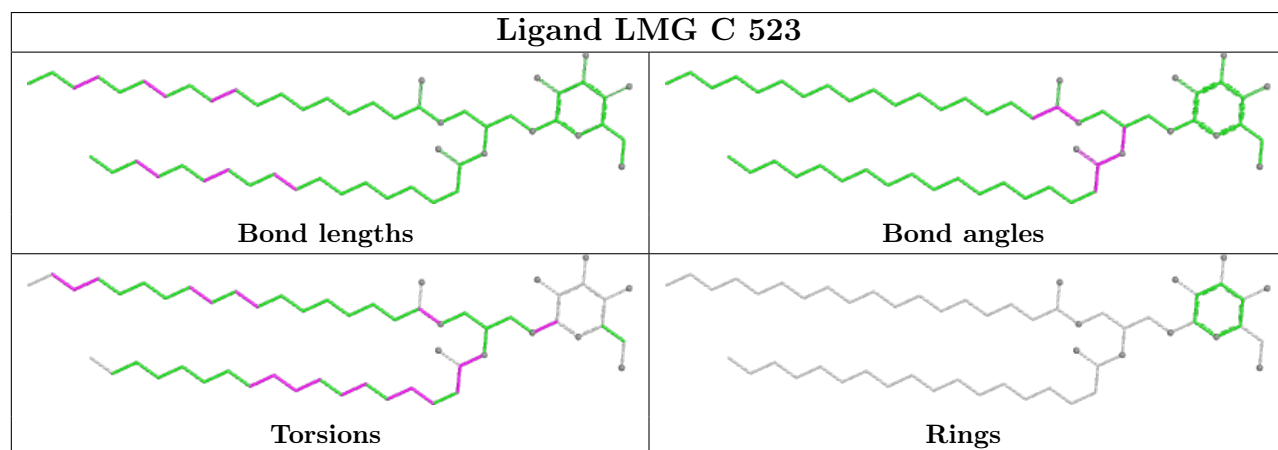
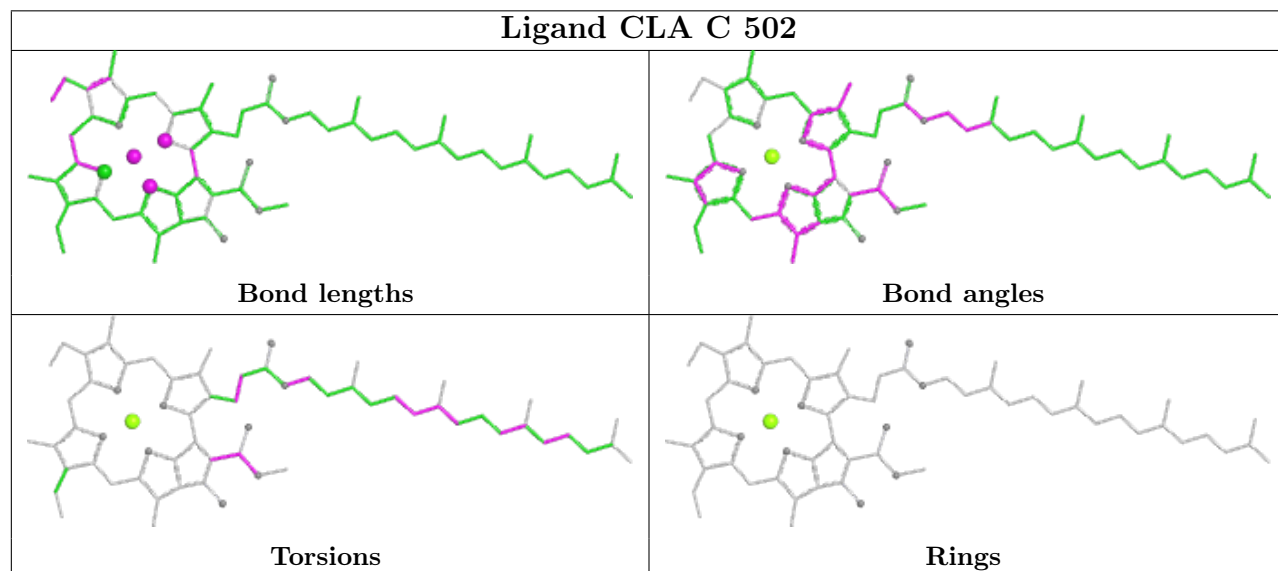
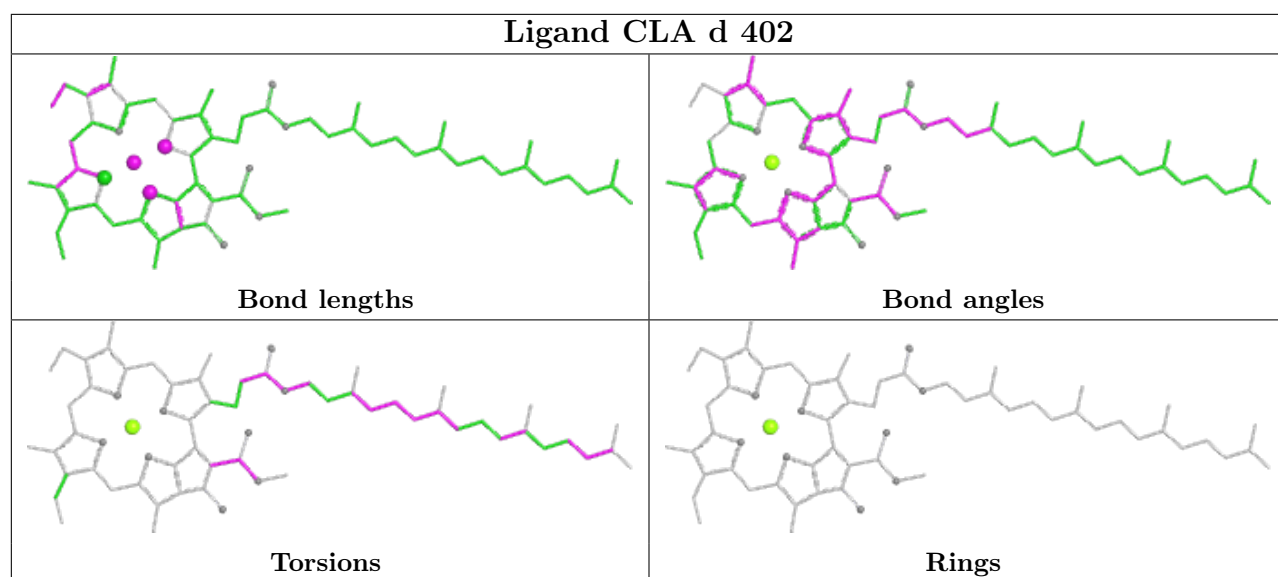


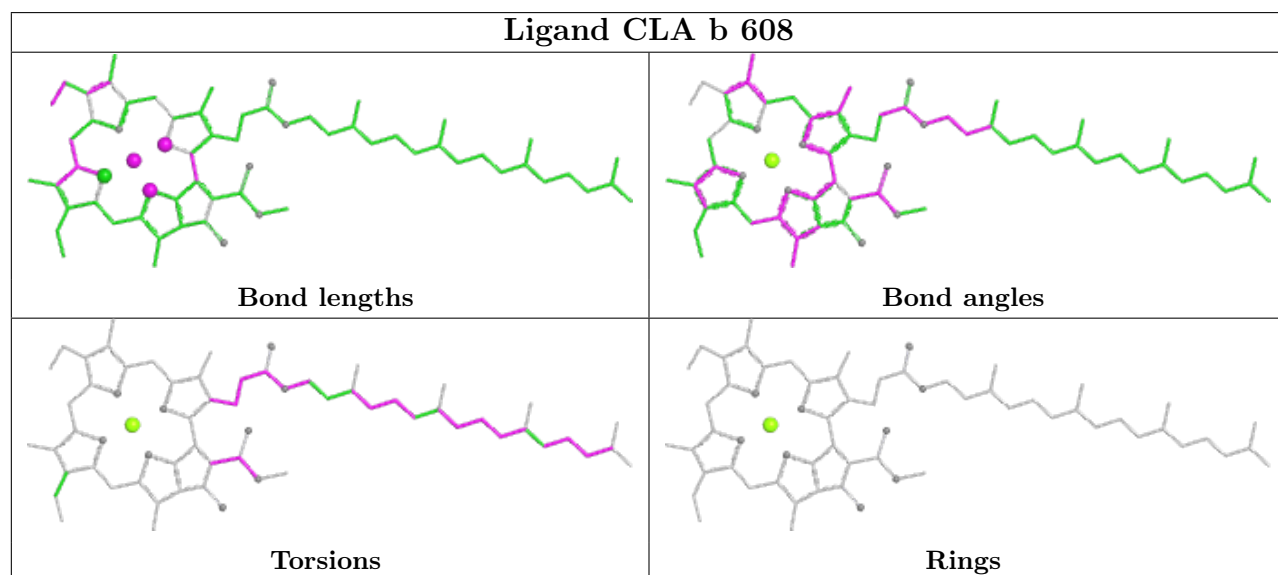
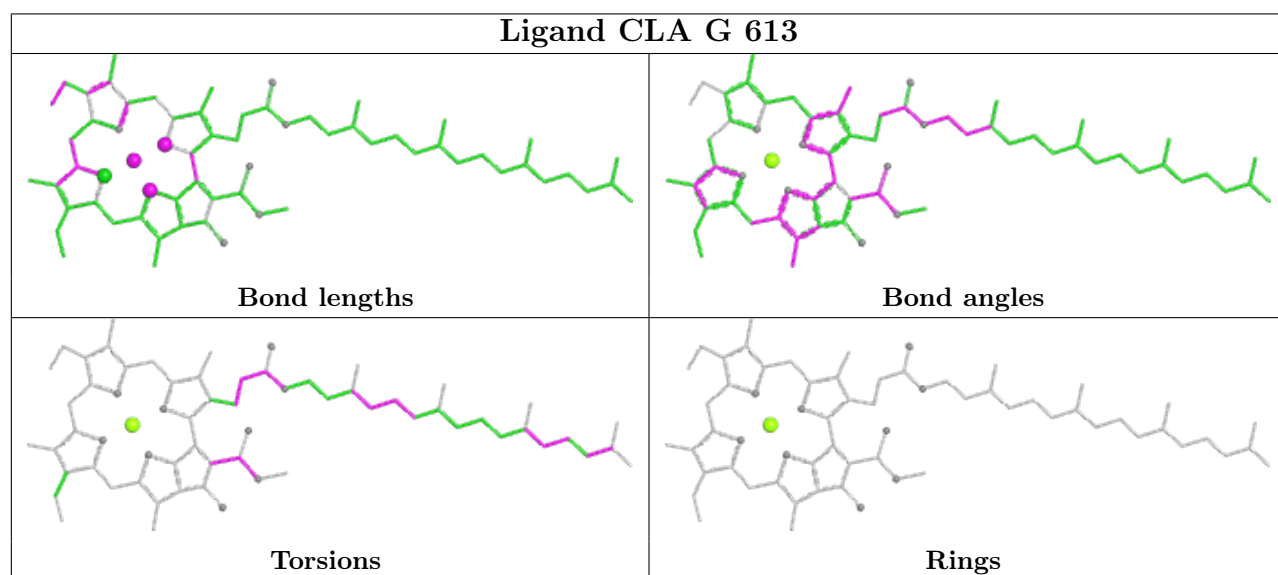
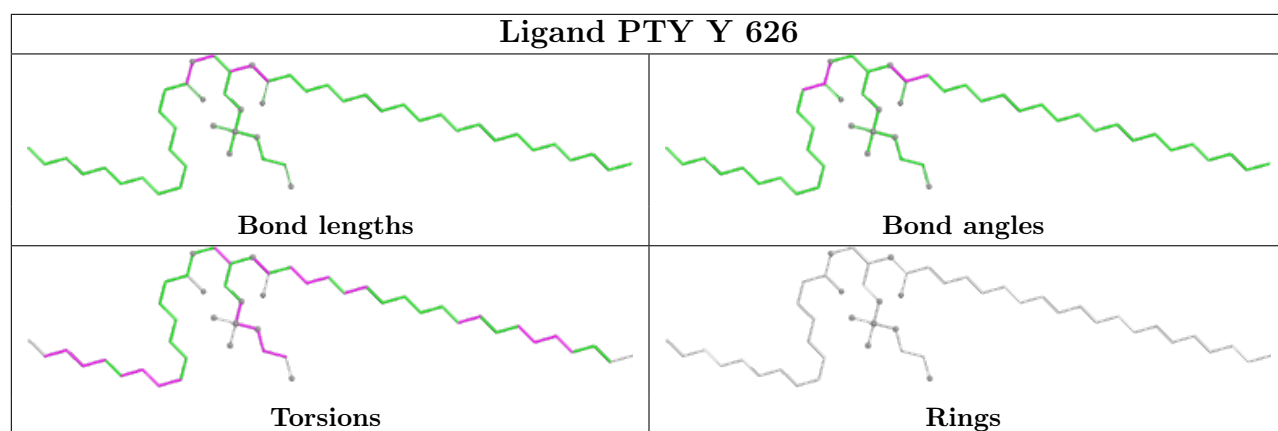


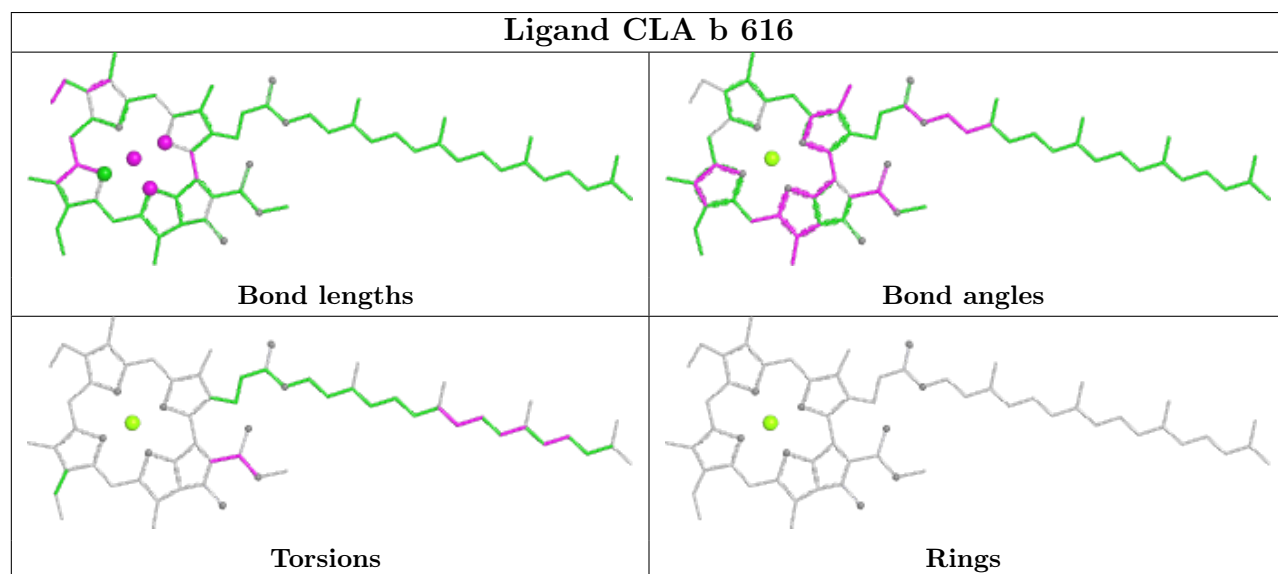
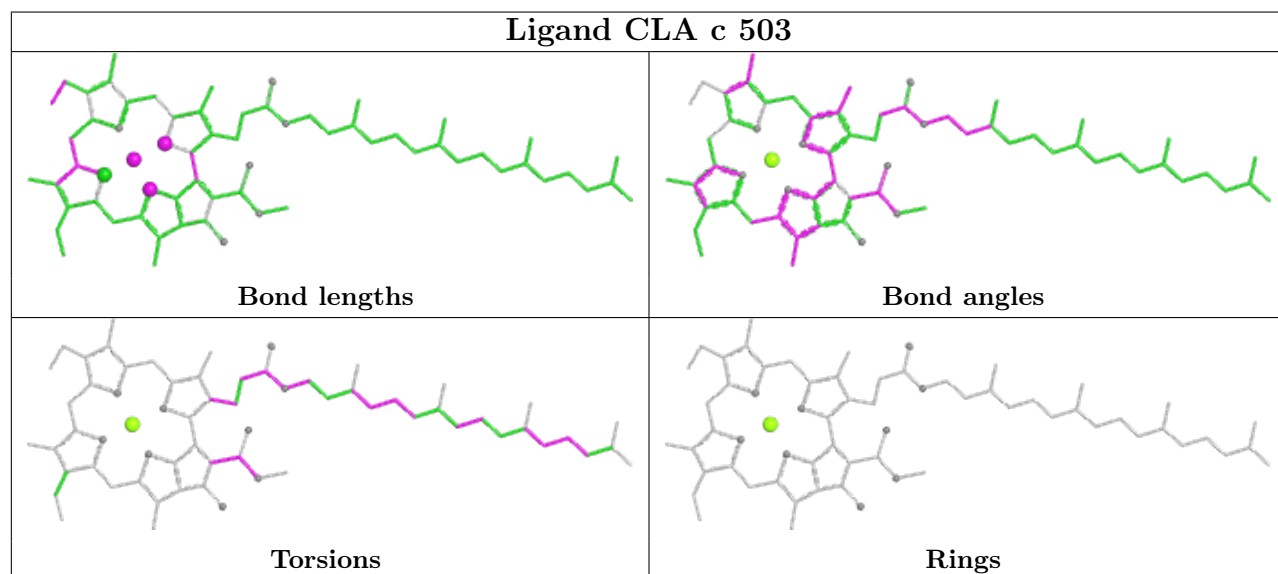
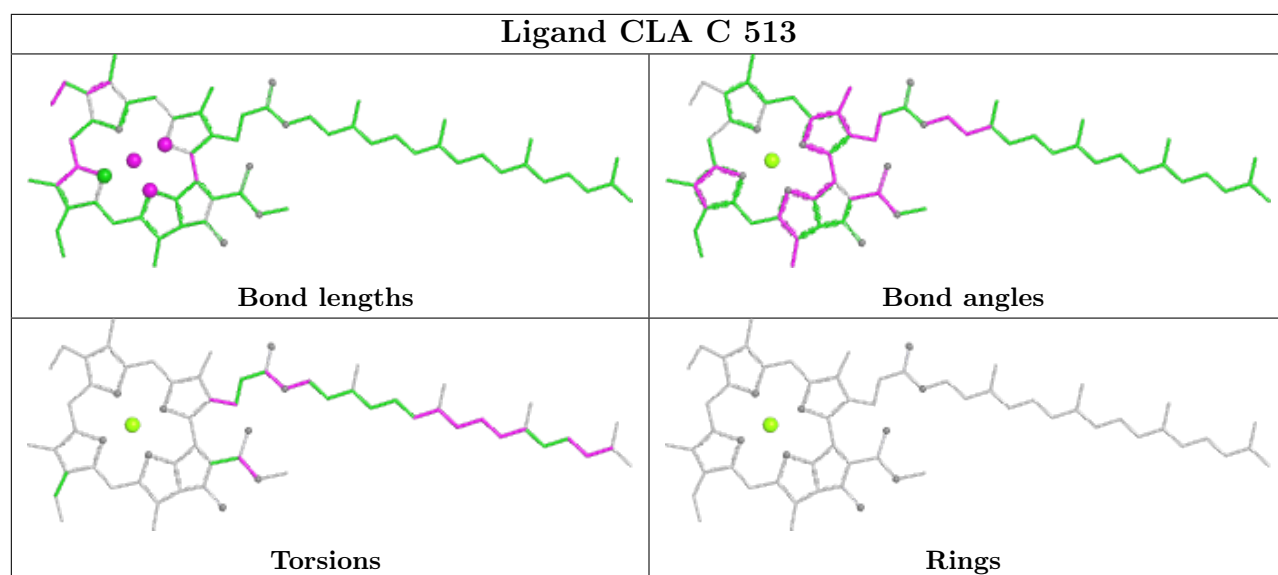


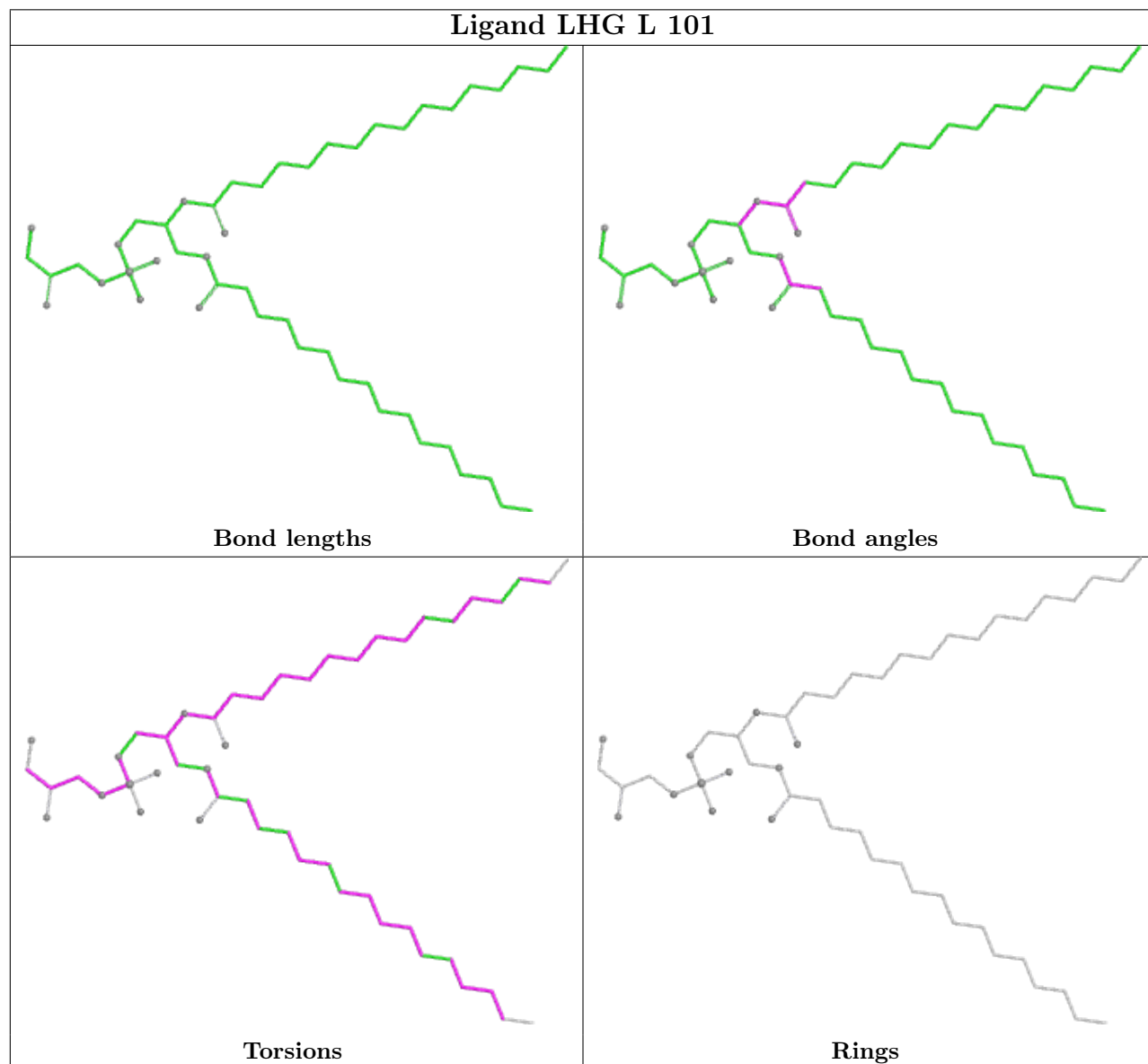
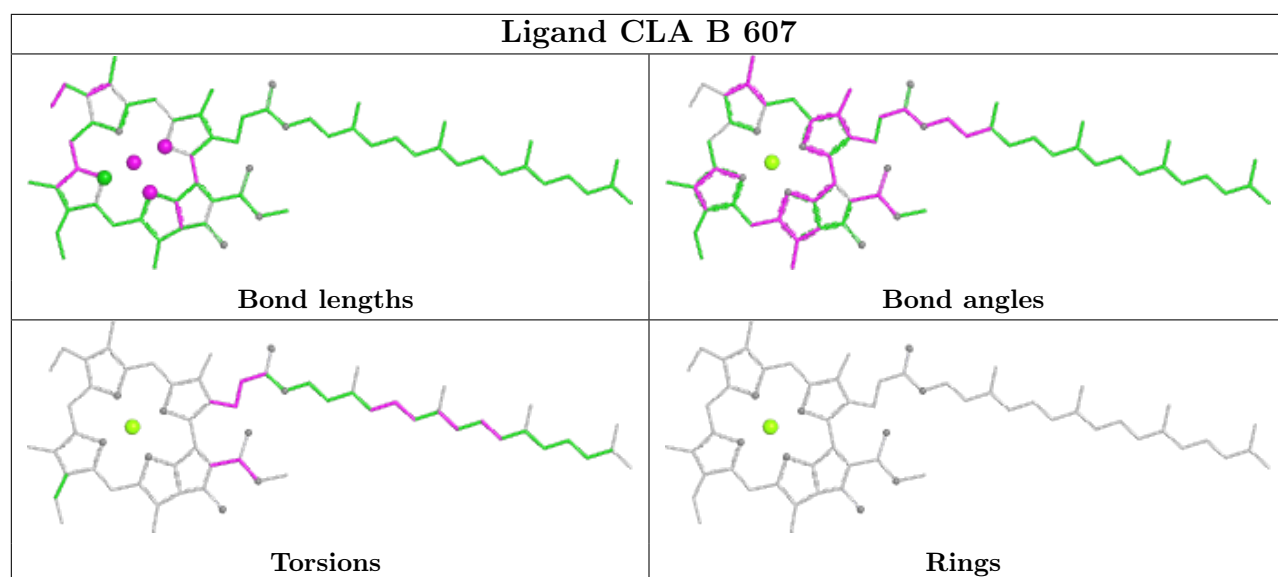




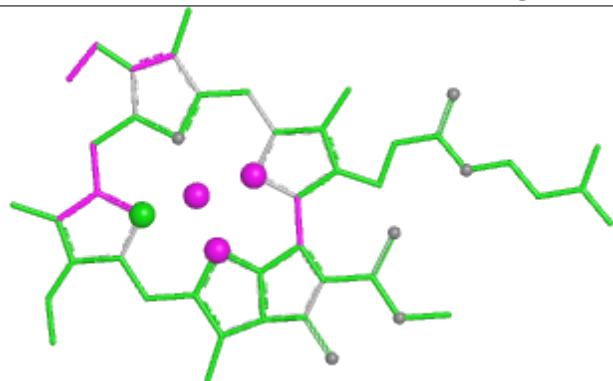




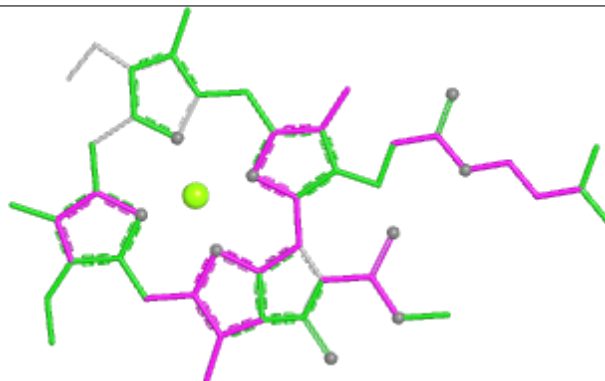




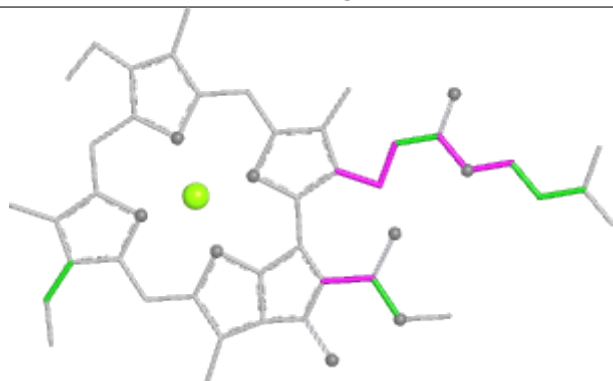
Ligand CLA A 407



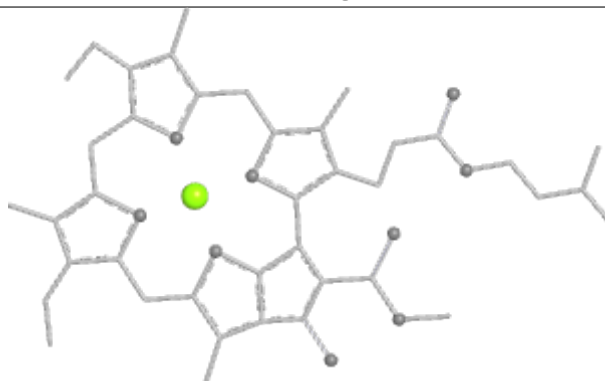
Bond lengths



Bond angles

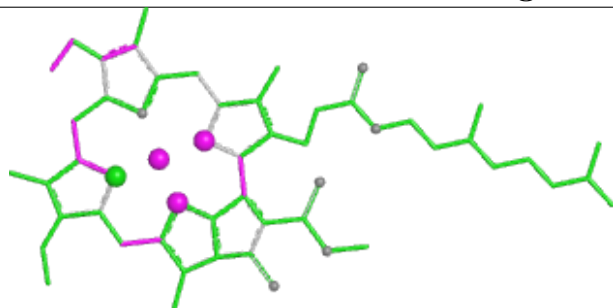


Torsions

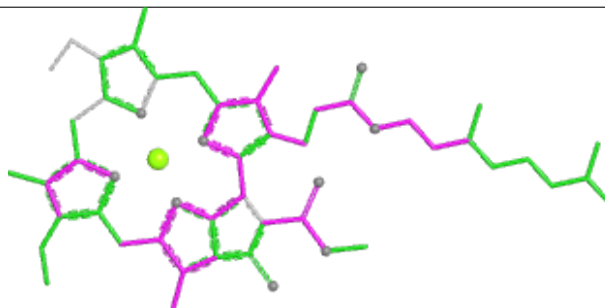


Rings

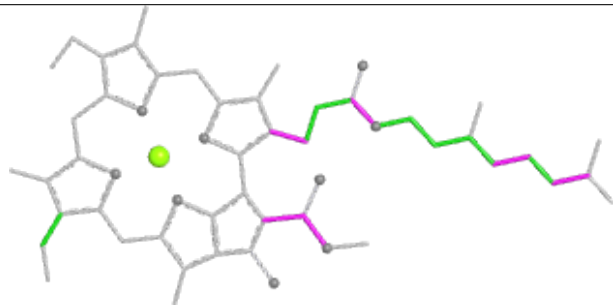
Ligand CLA S 604



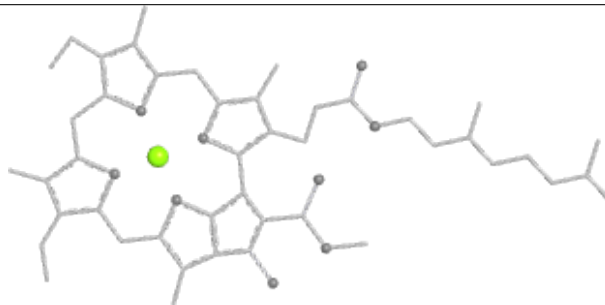
Bond lengths



Bond angles

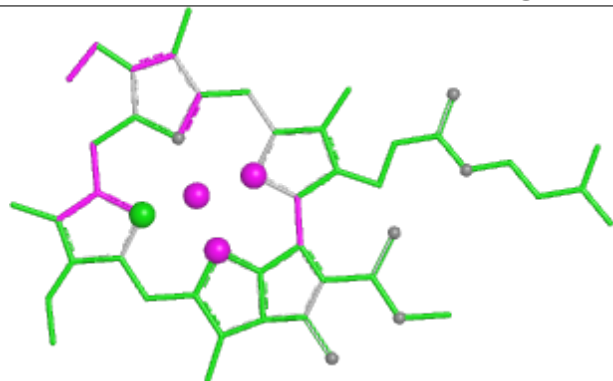


Torsions

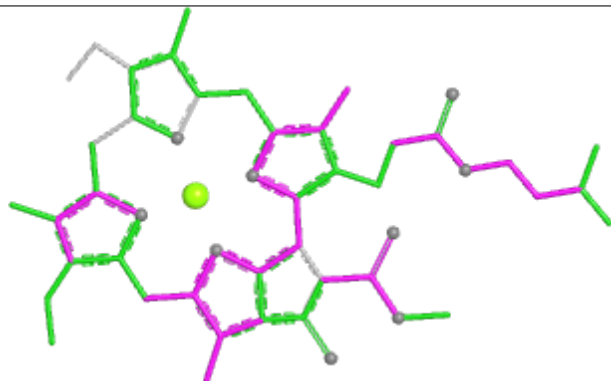


Rings

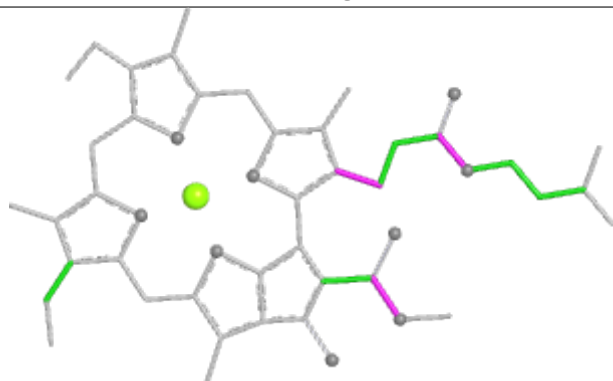
Ligand CLA S 617



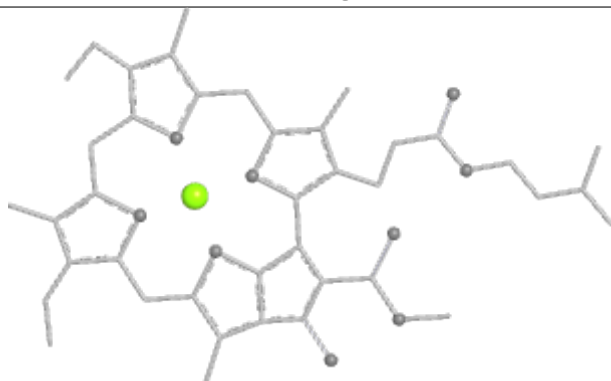
Bond lengths



Bond angles

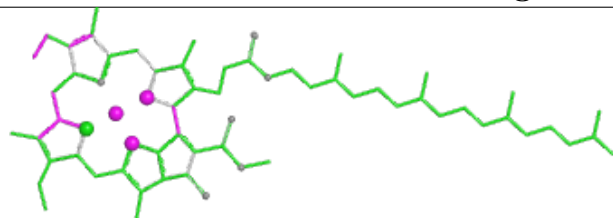


Torsions

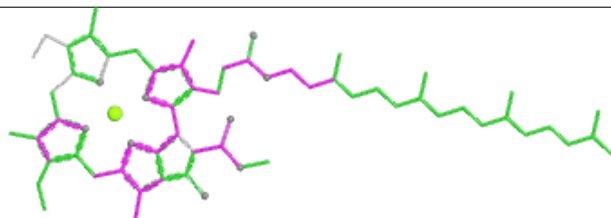


Rings

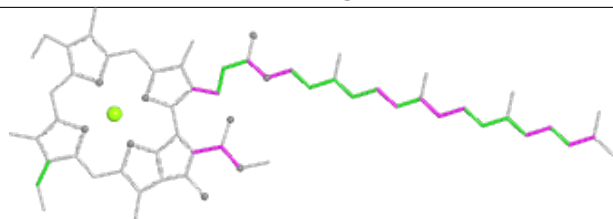
Ligand CLA Y 614



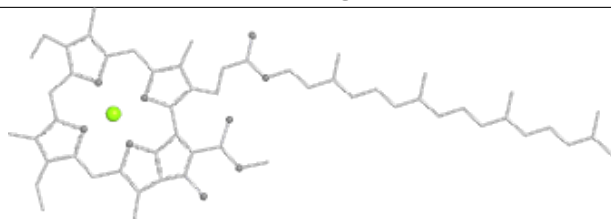
Bond lengths



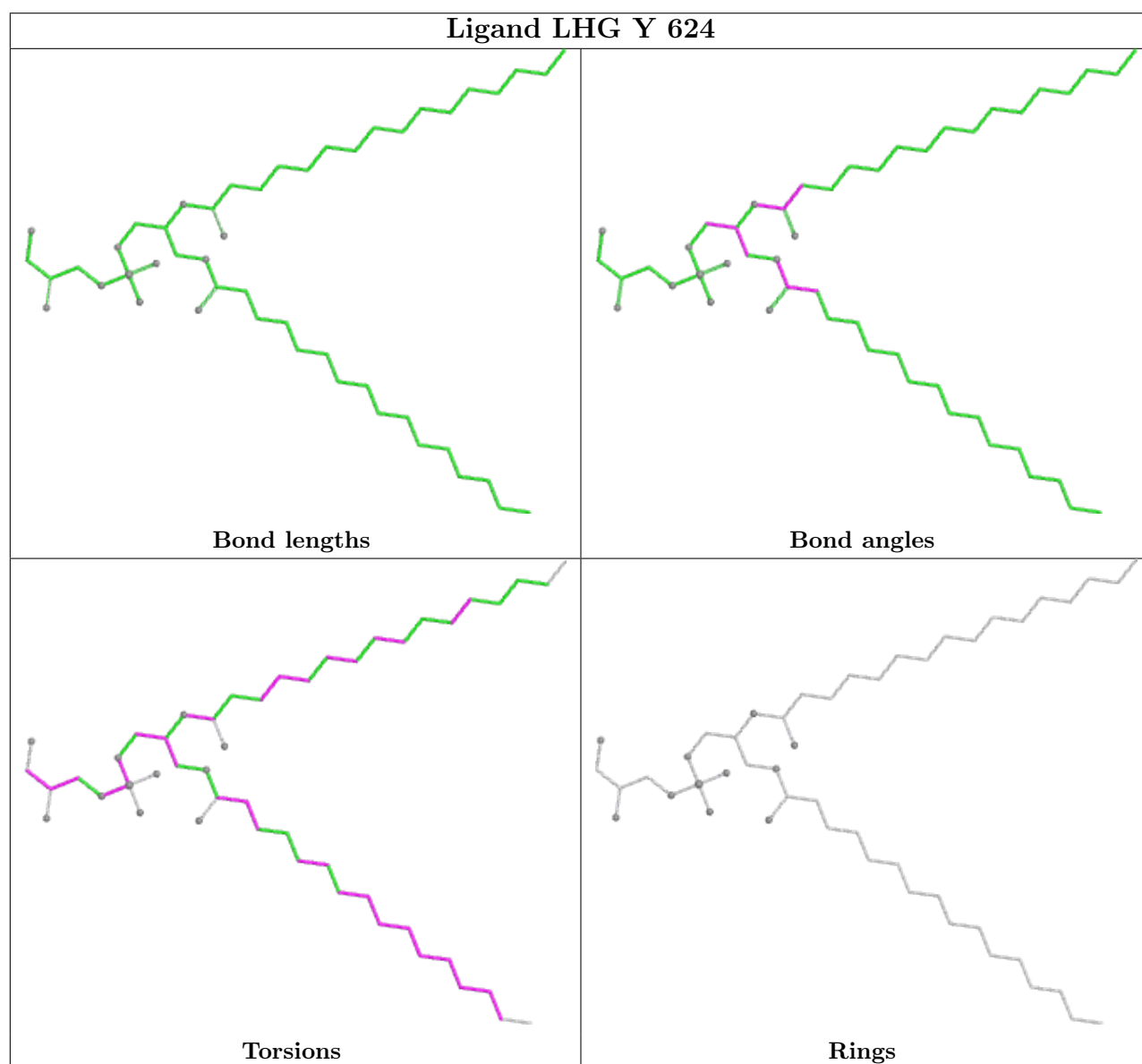
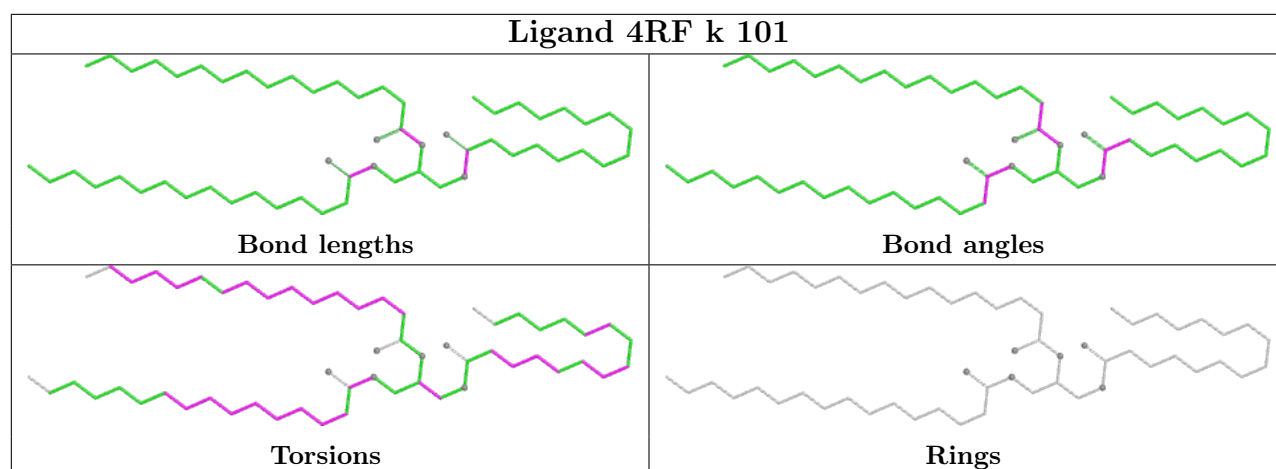
Bond angles

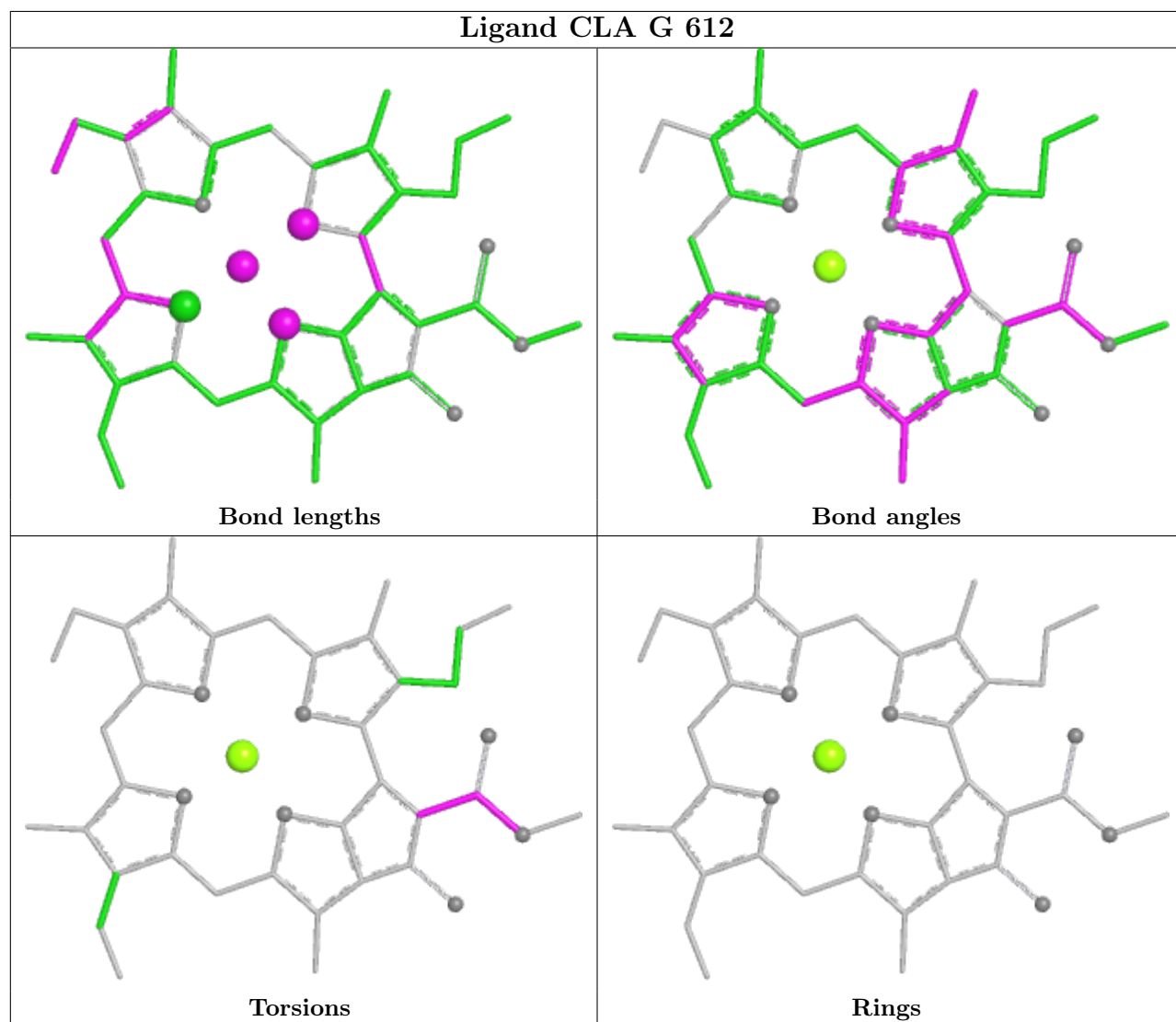
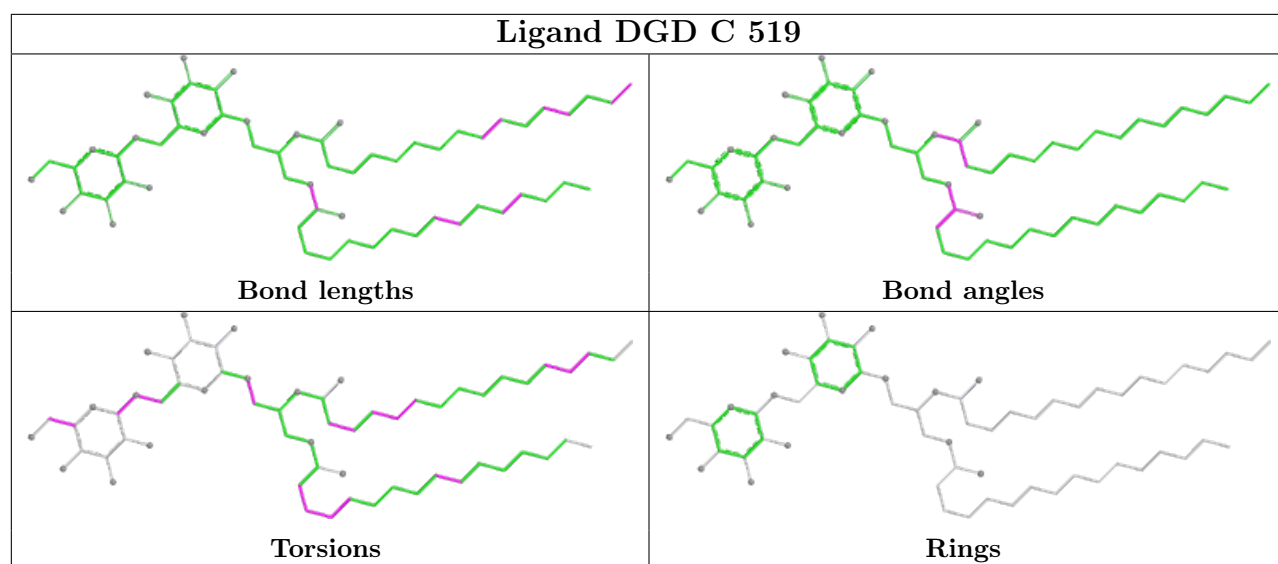


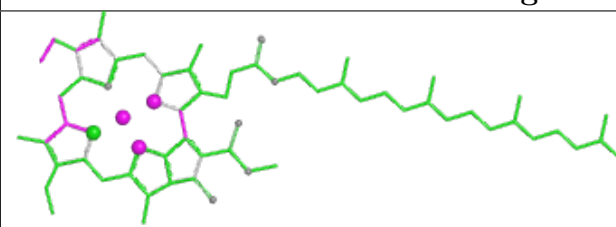
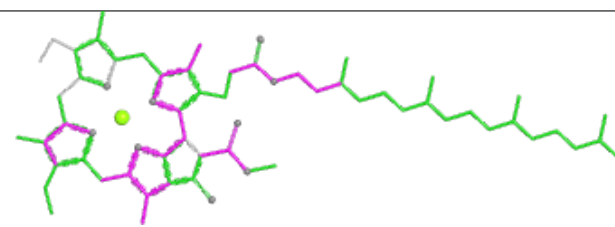
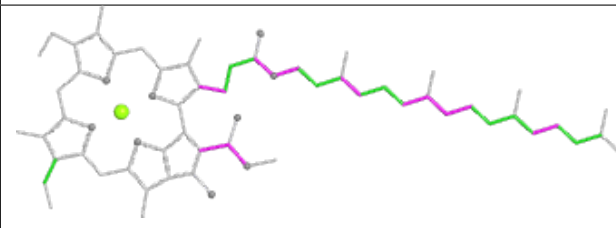
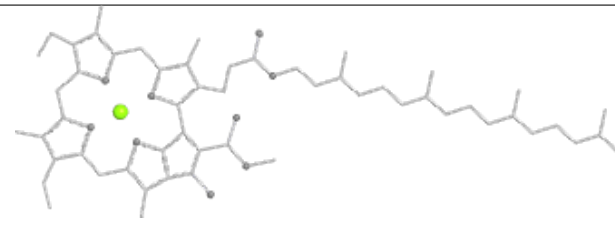
Torsions

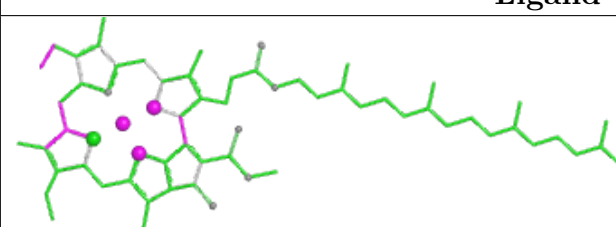
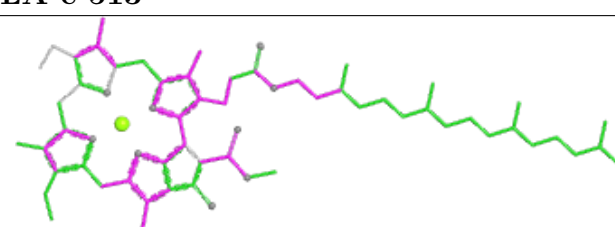
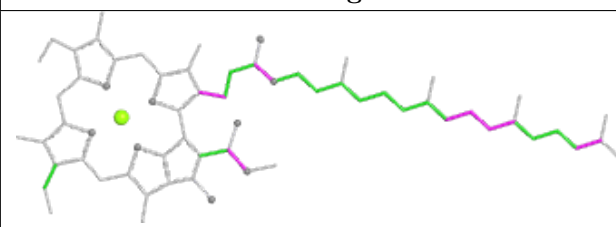
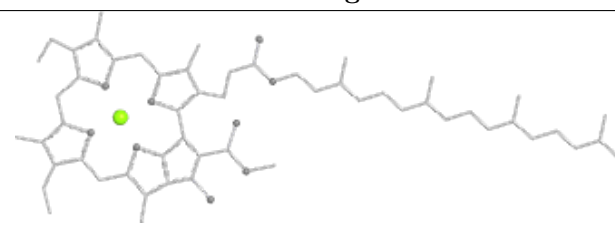


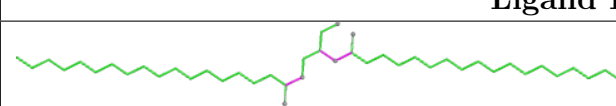
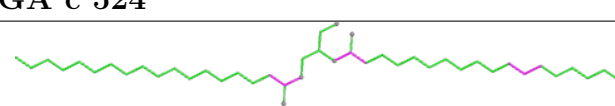
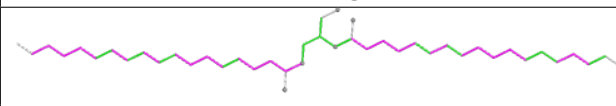
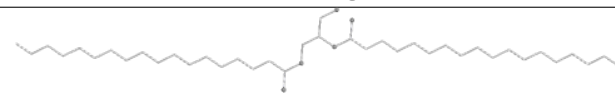
Rings

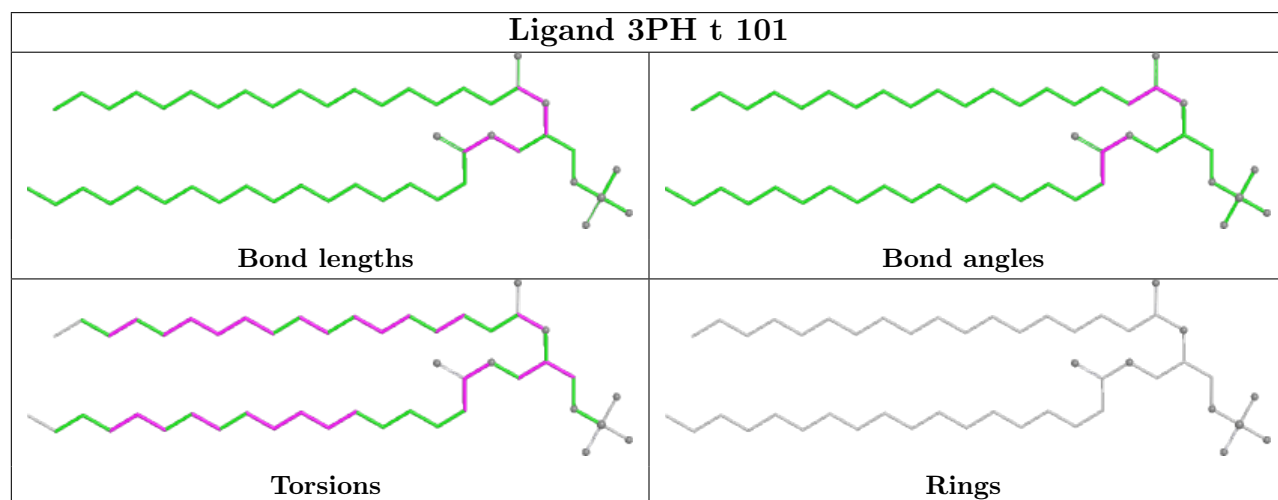
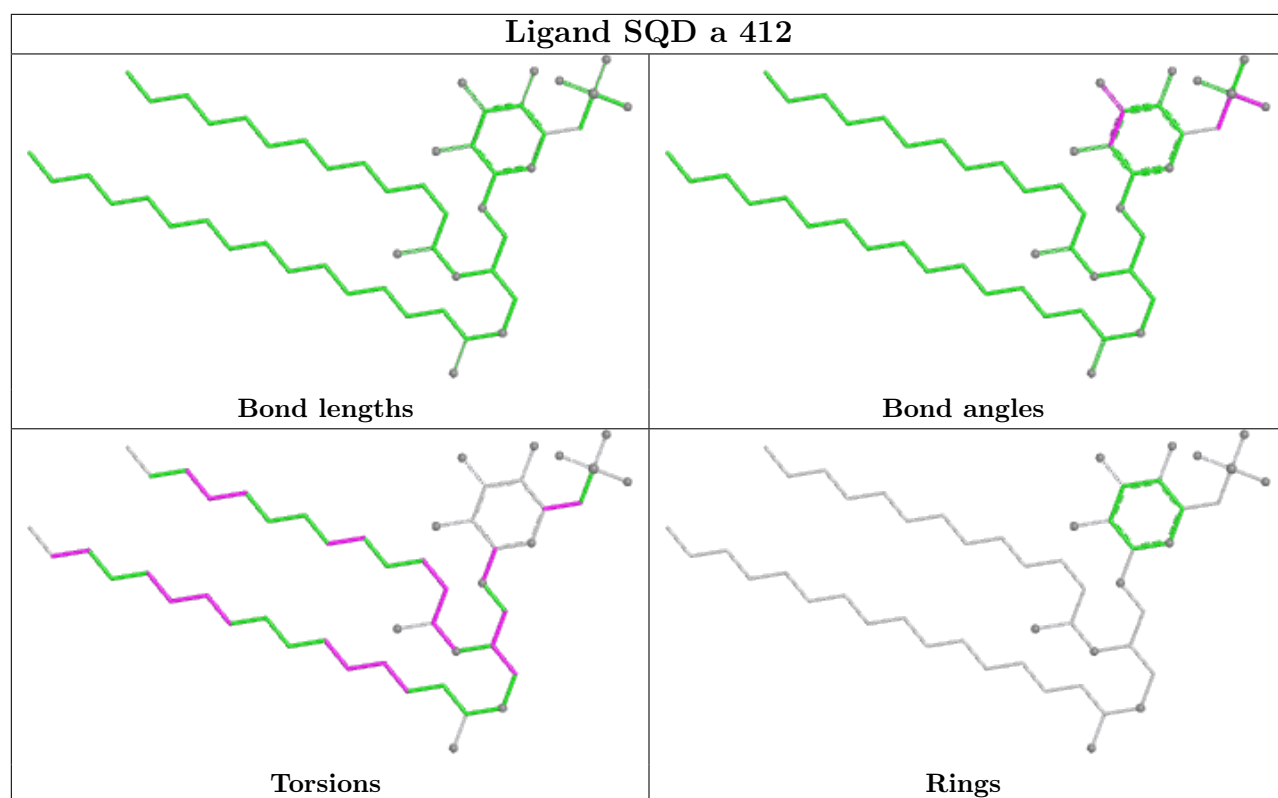


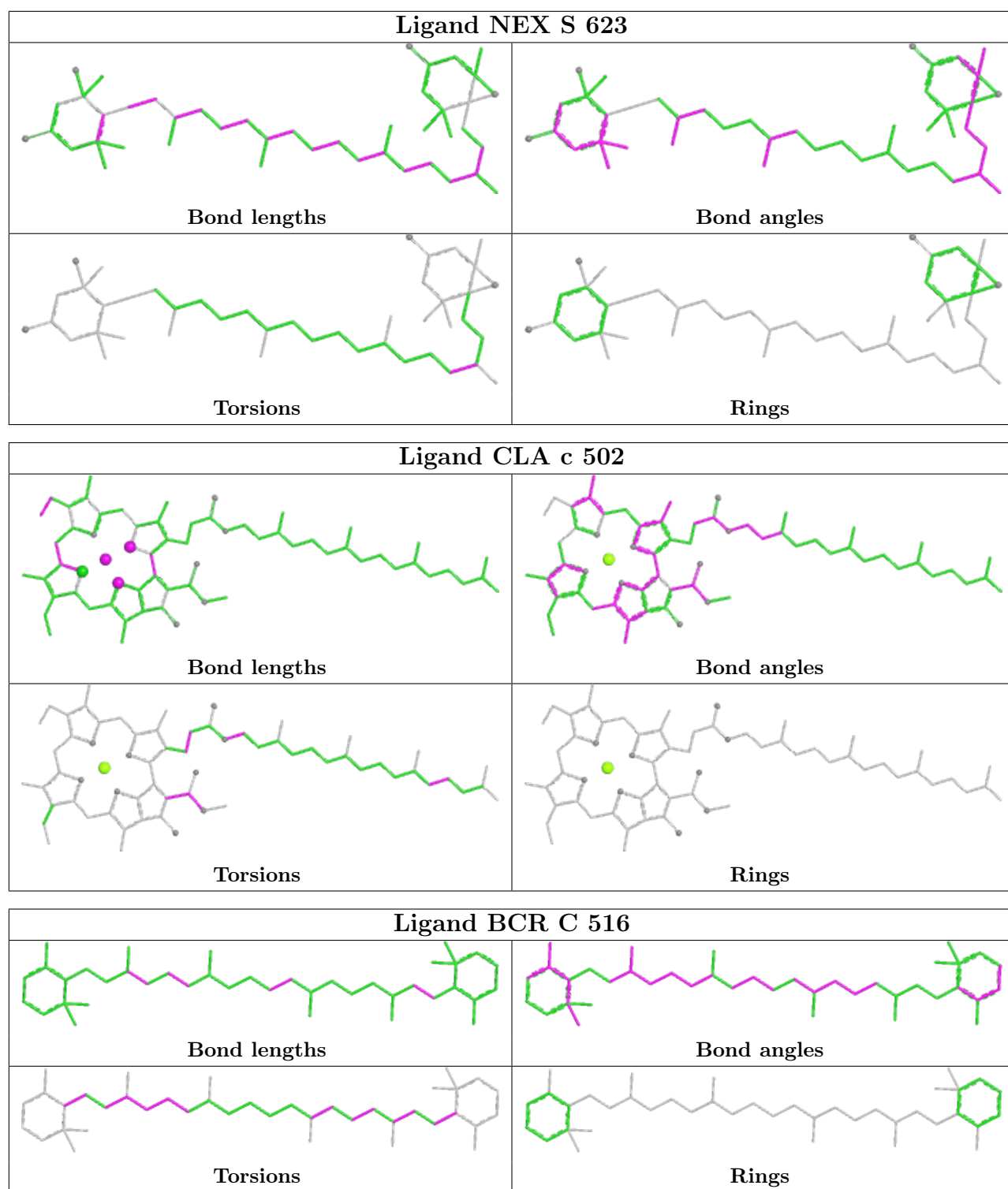


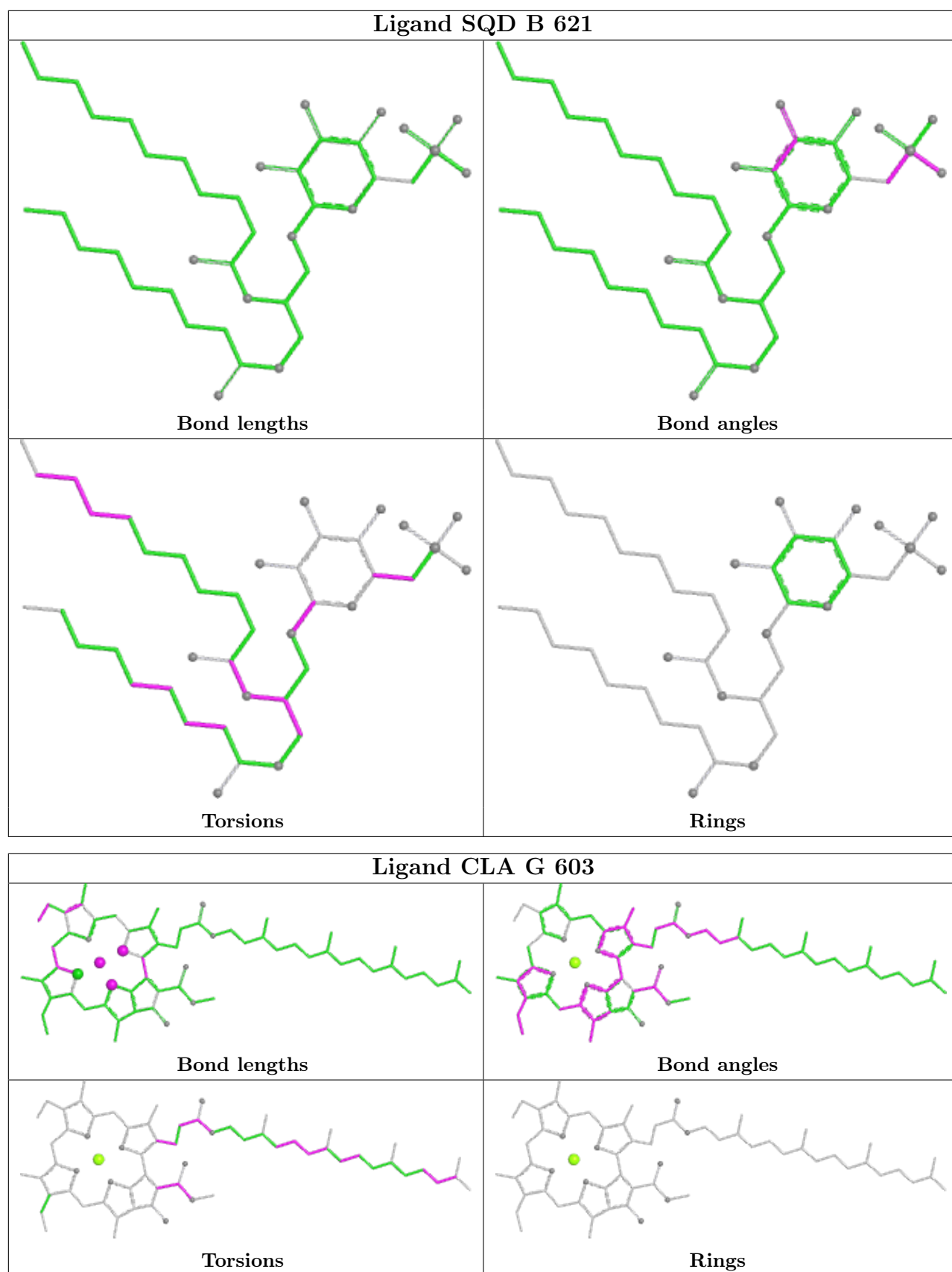
Ligand CLA Y 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

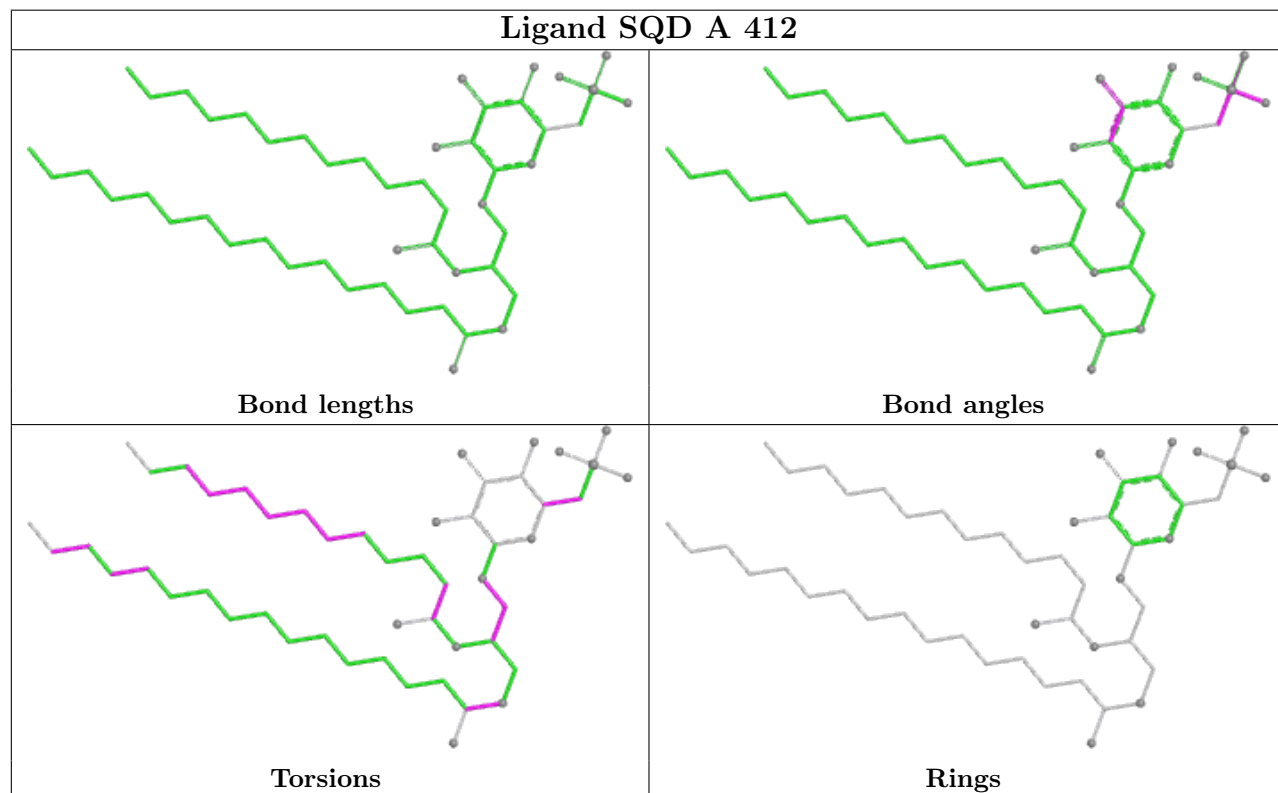
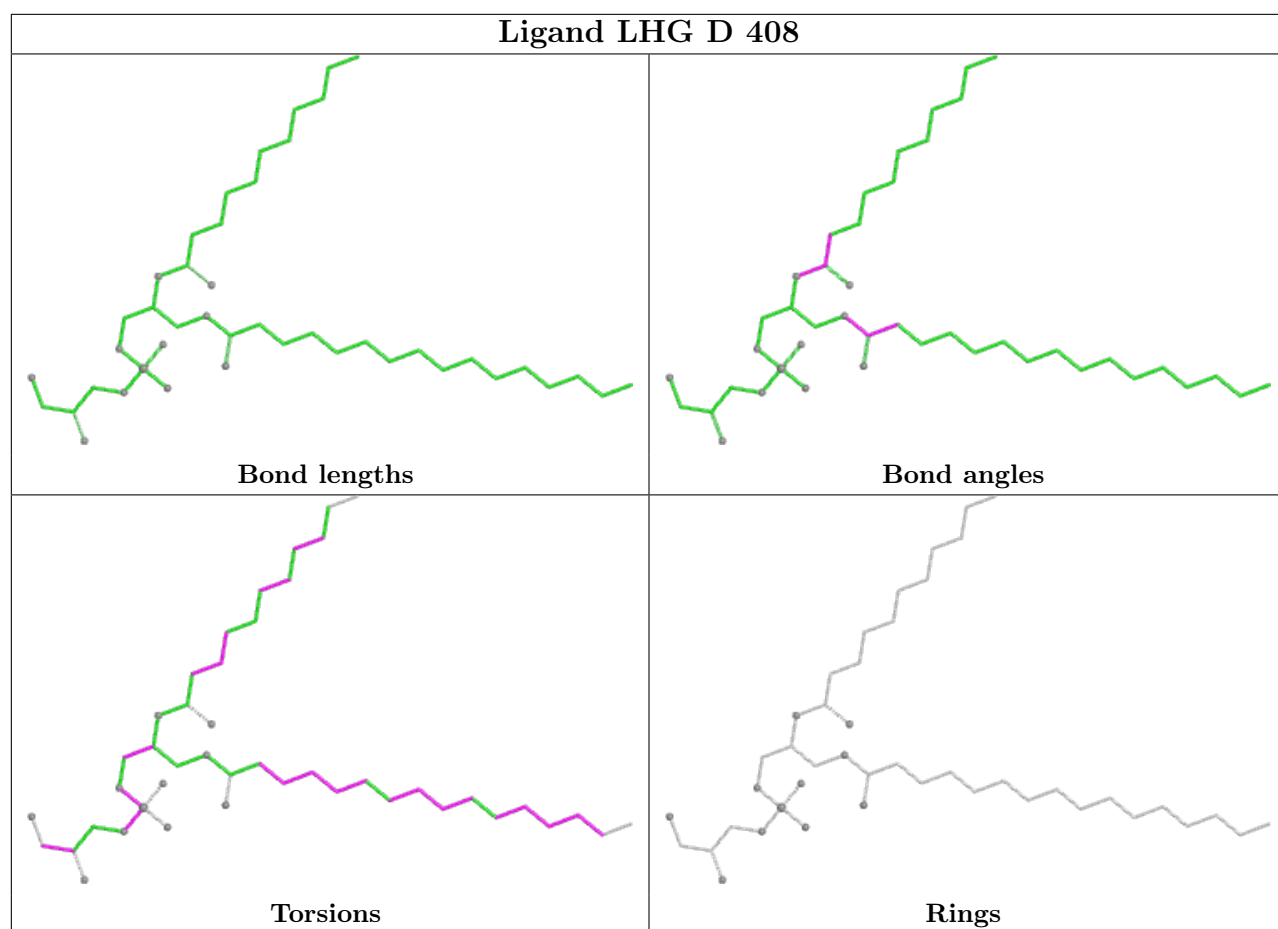
Ligand CLA c 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

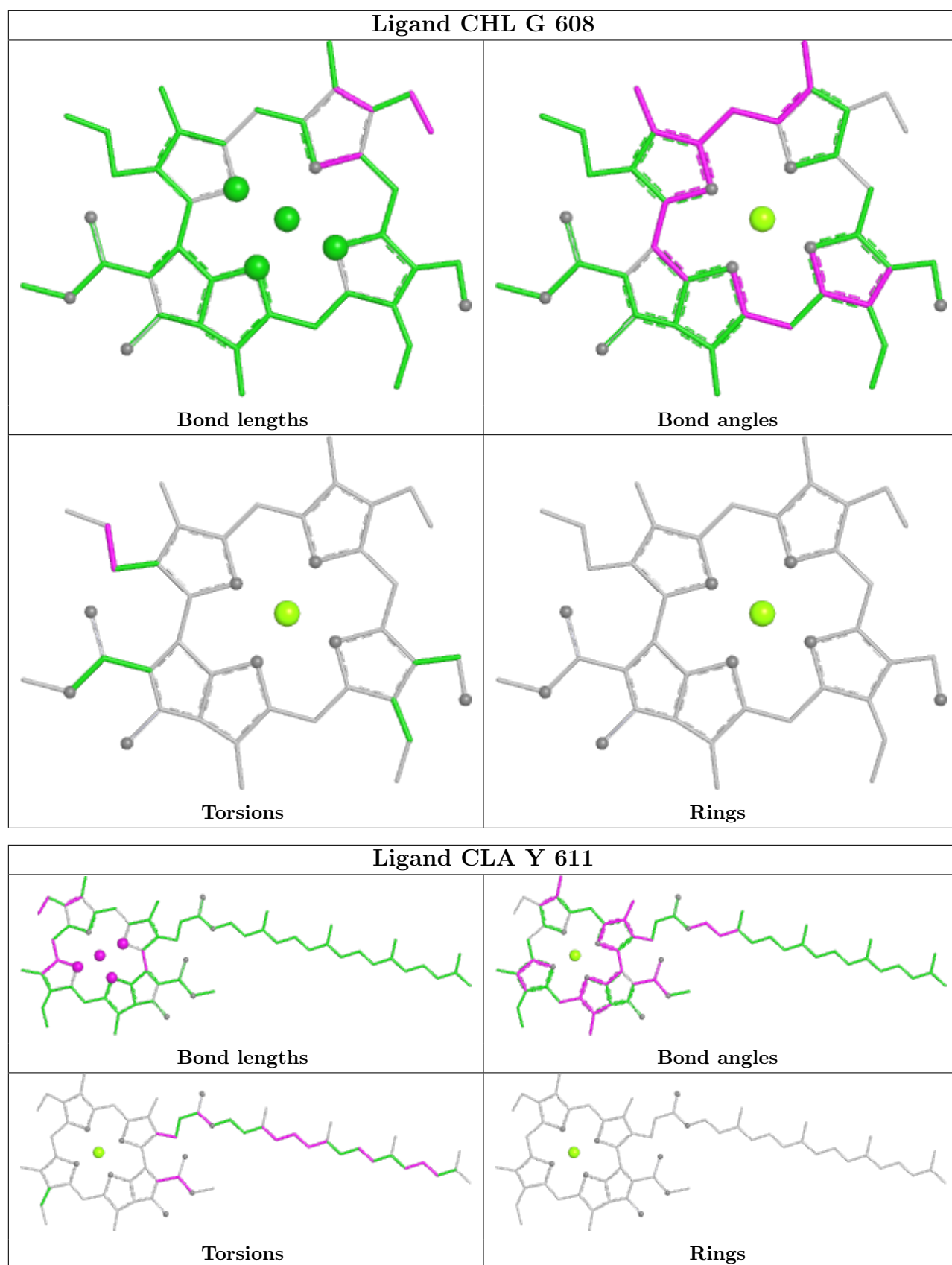
Ligand DGA c 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

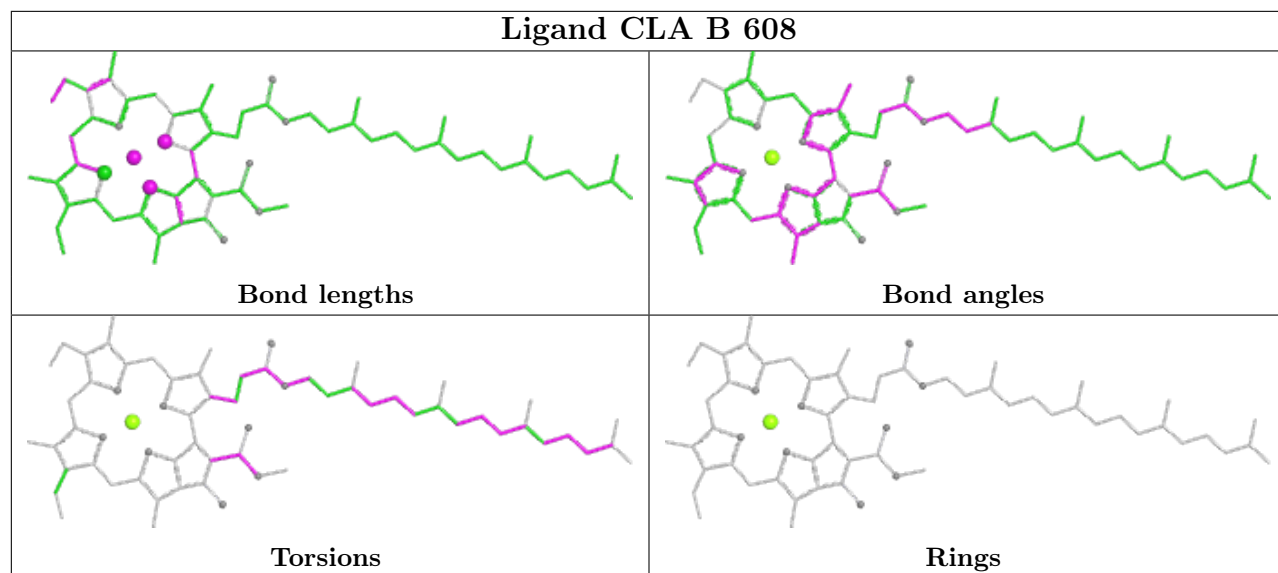
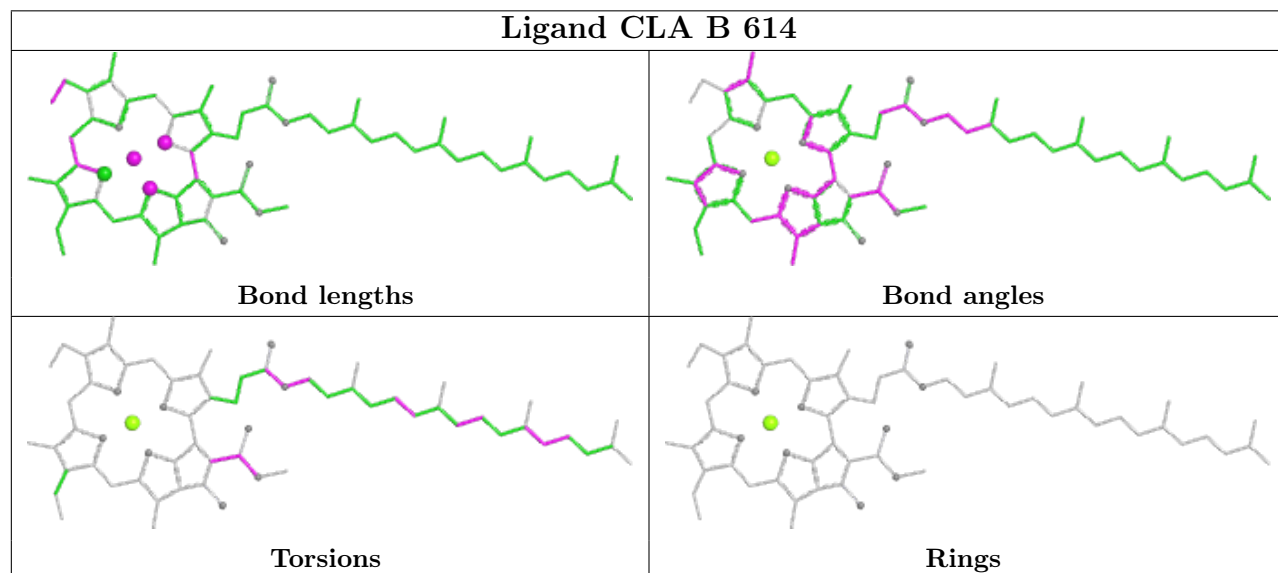
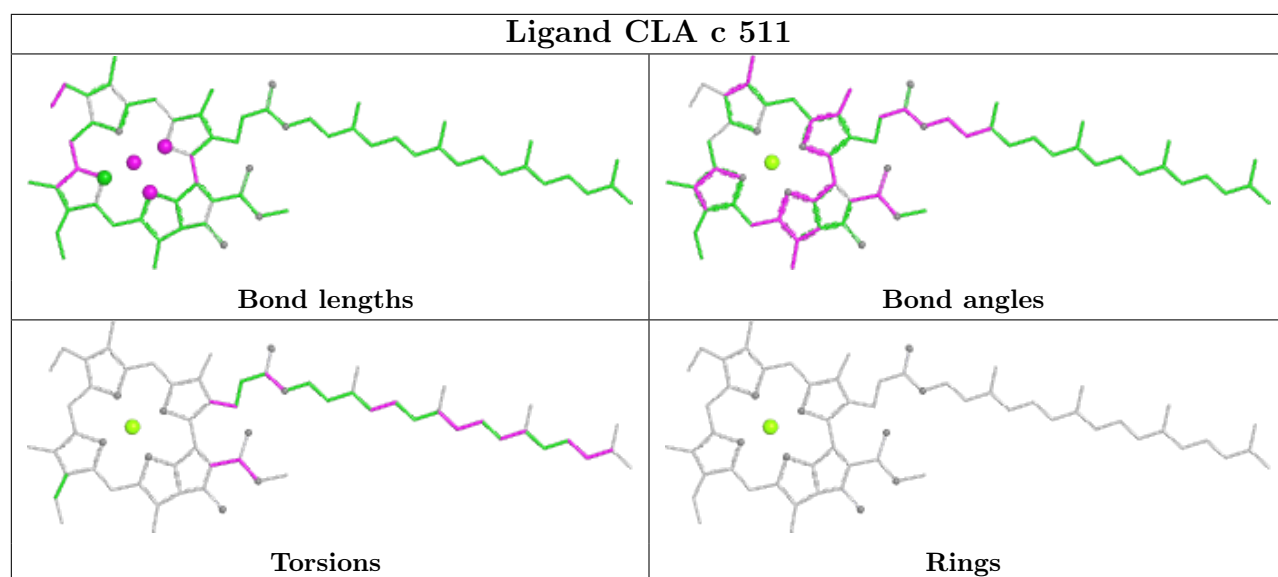


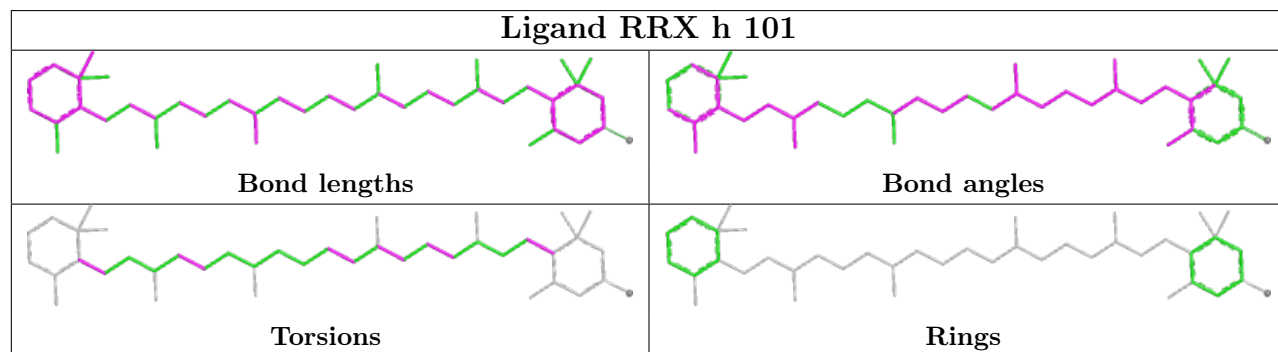
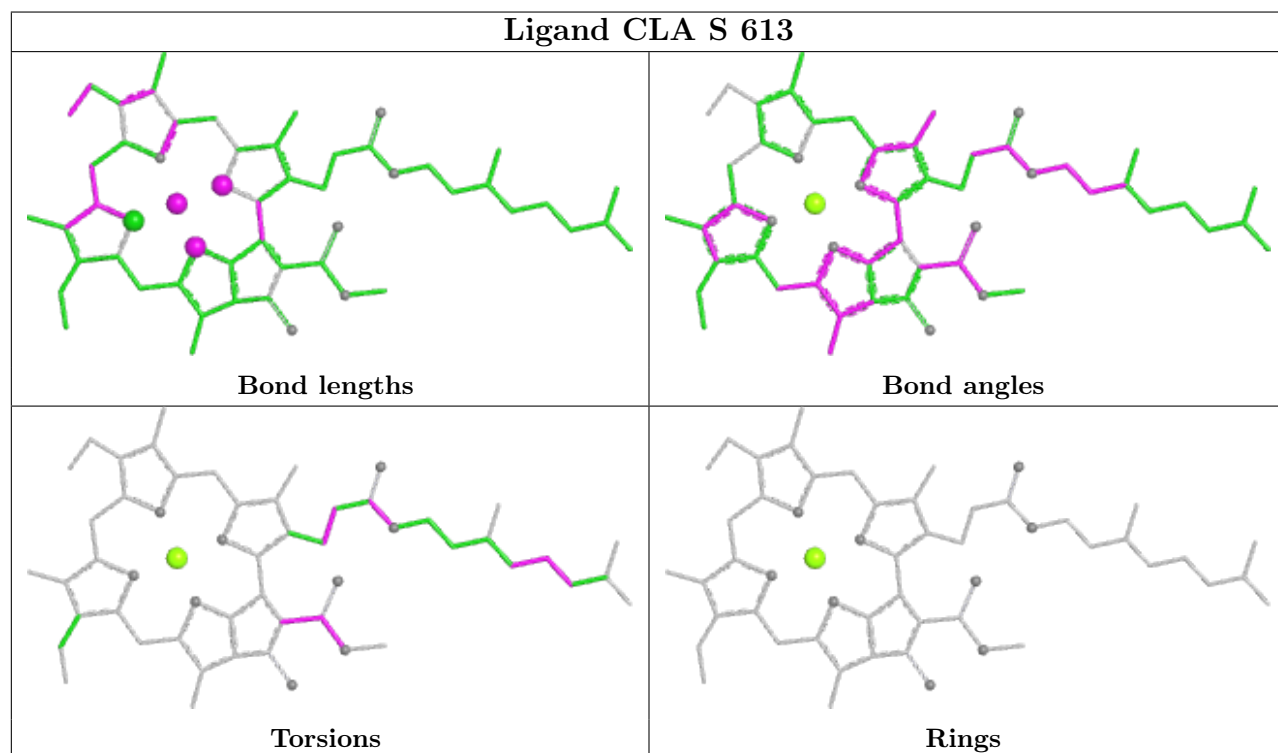
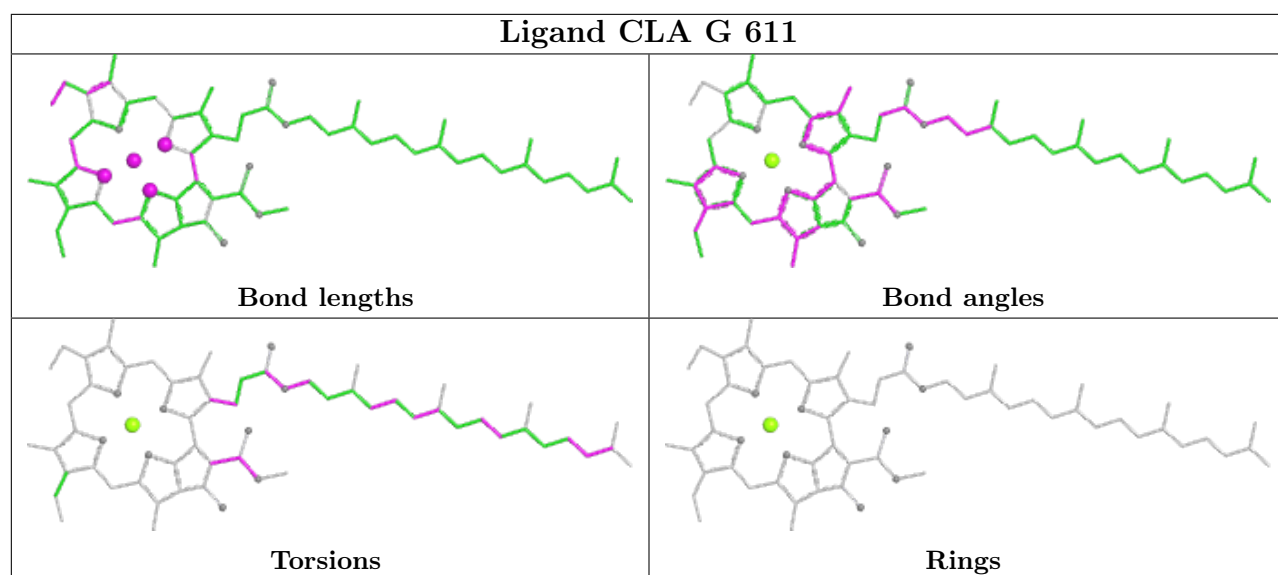


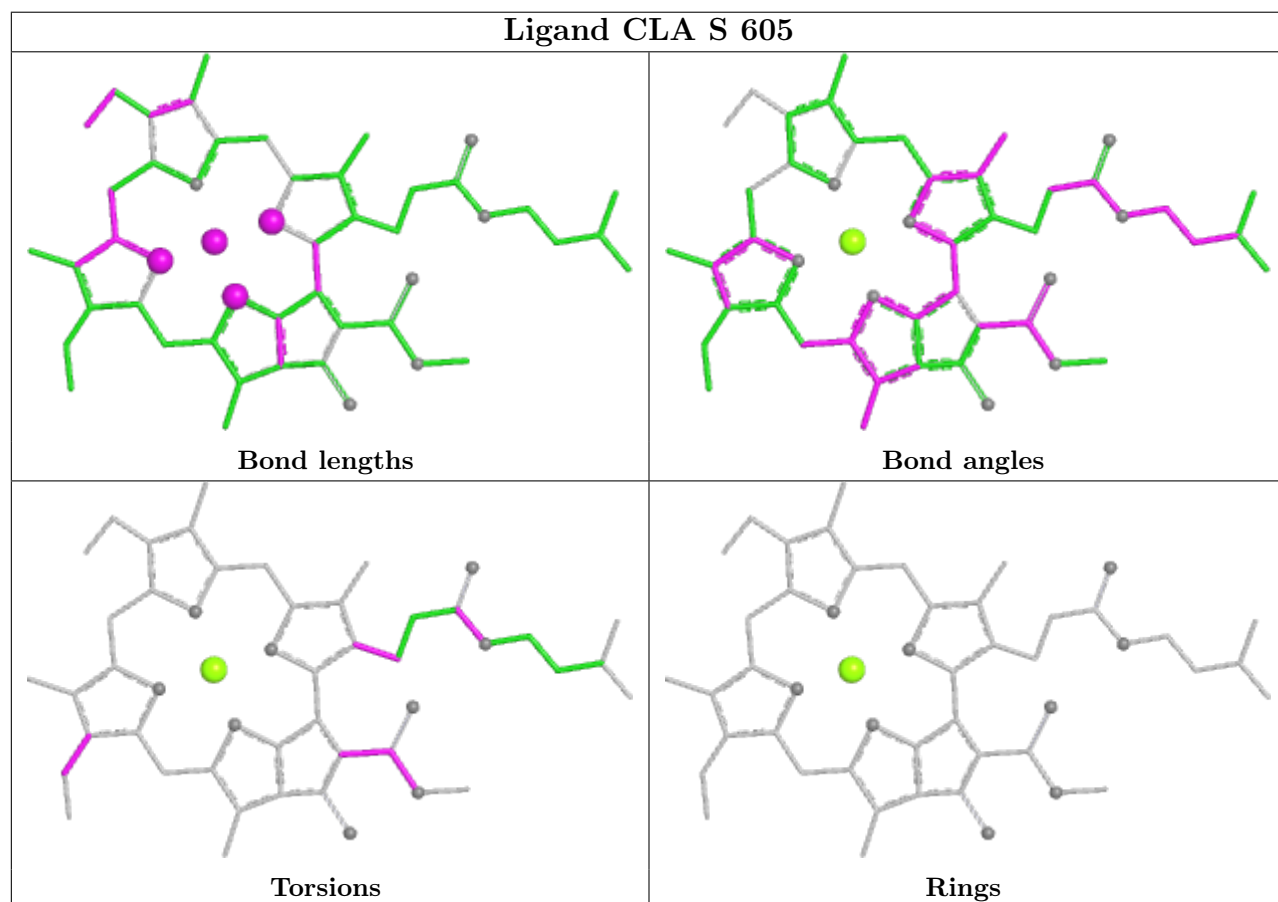
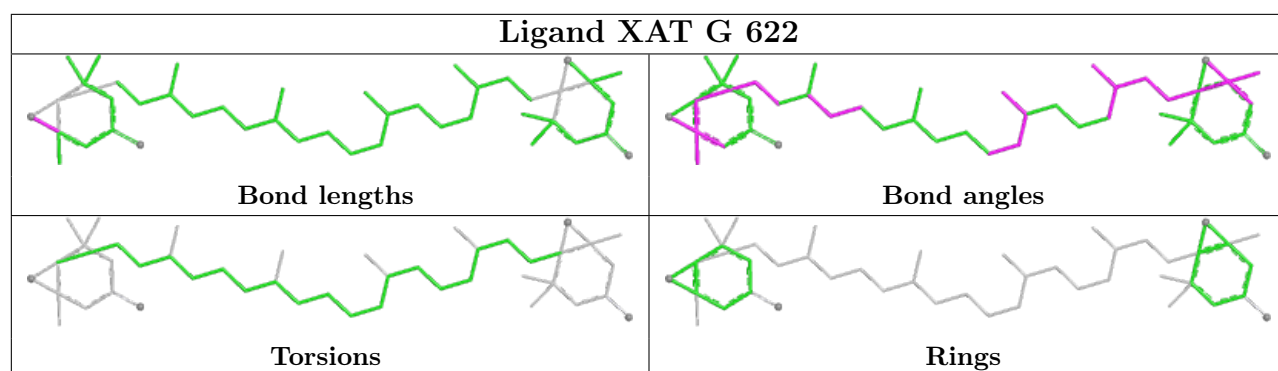


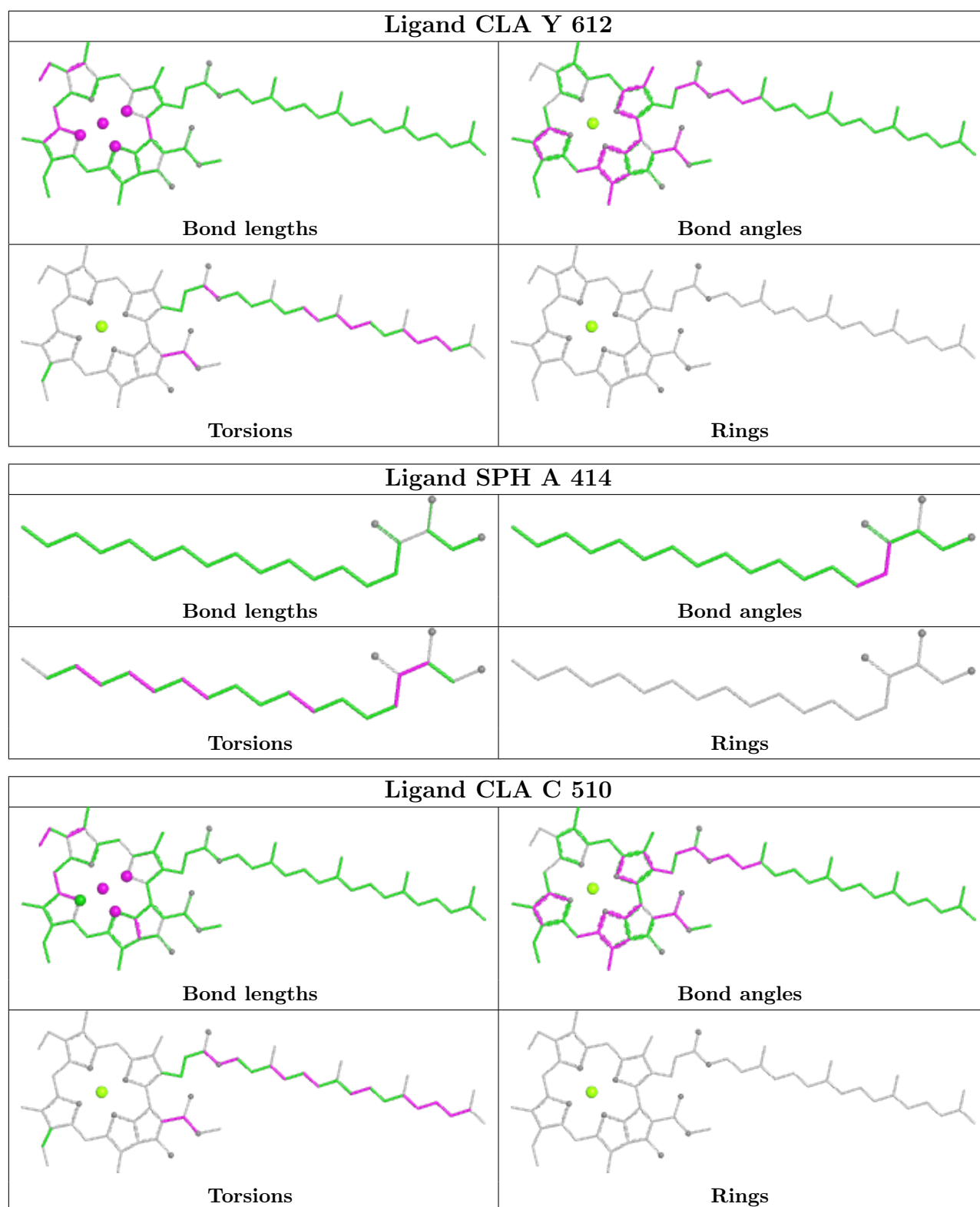


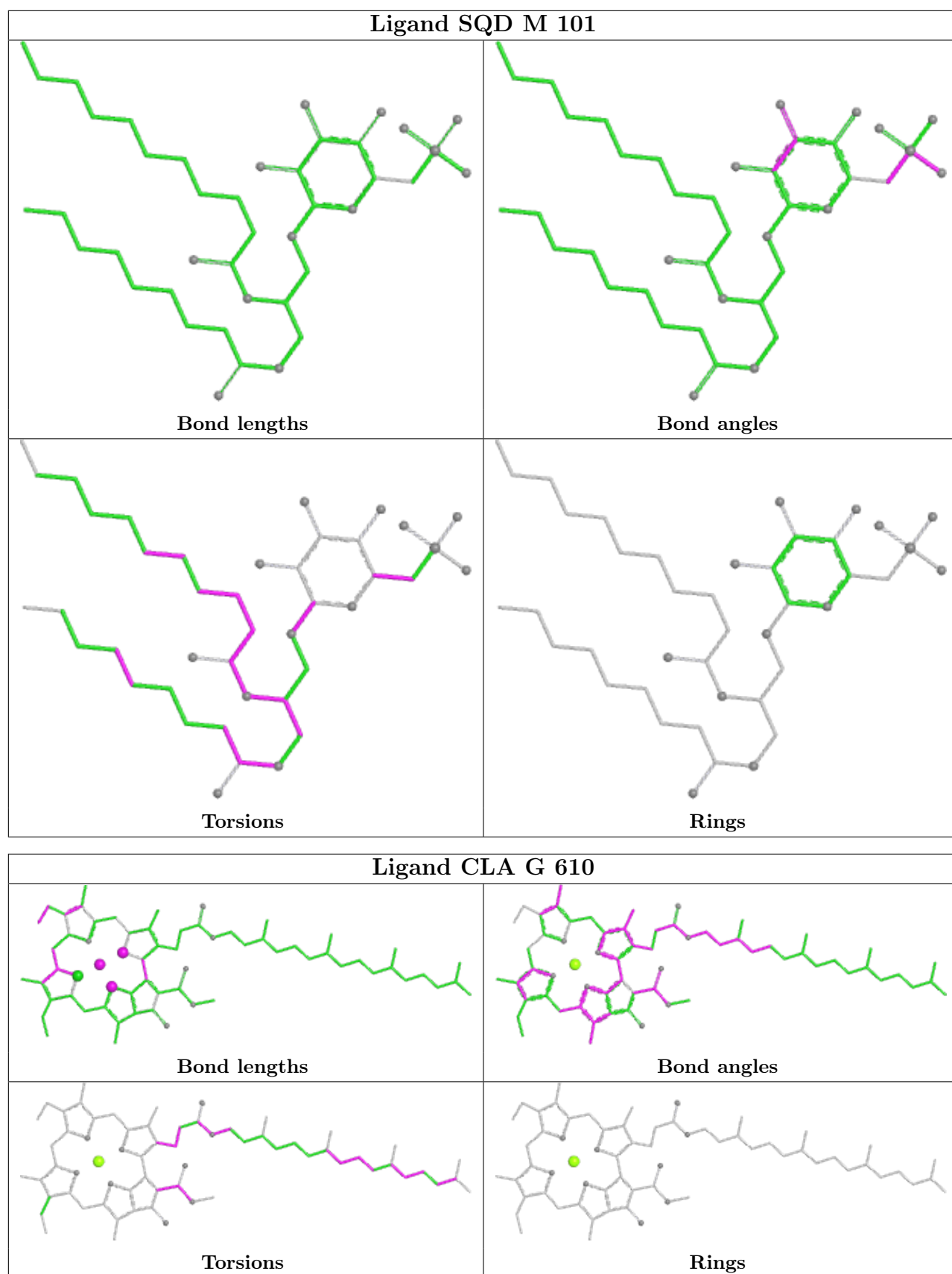


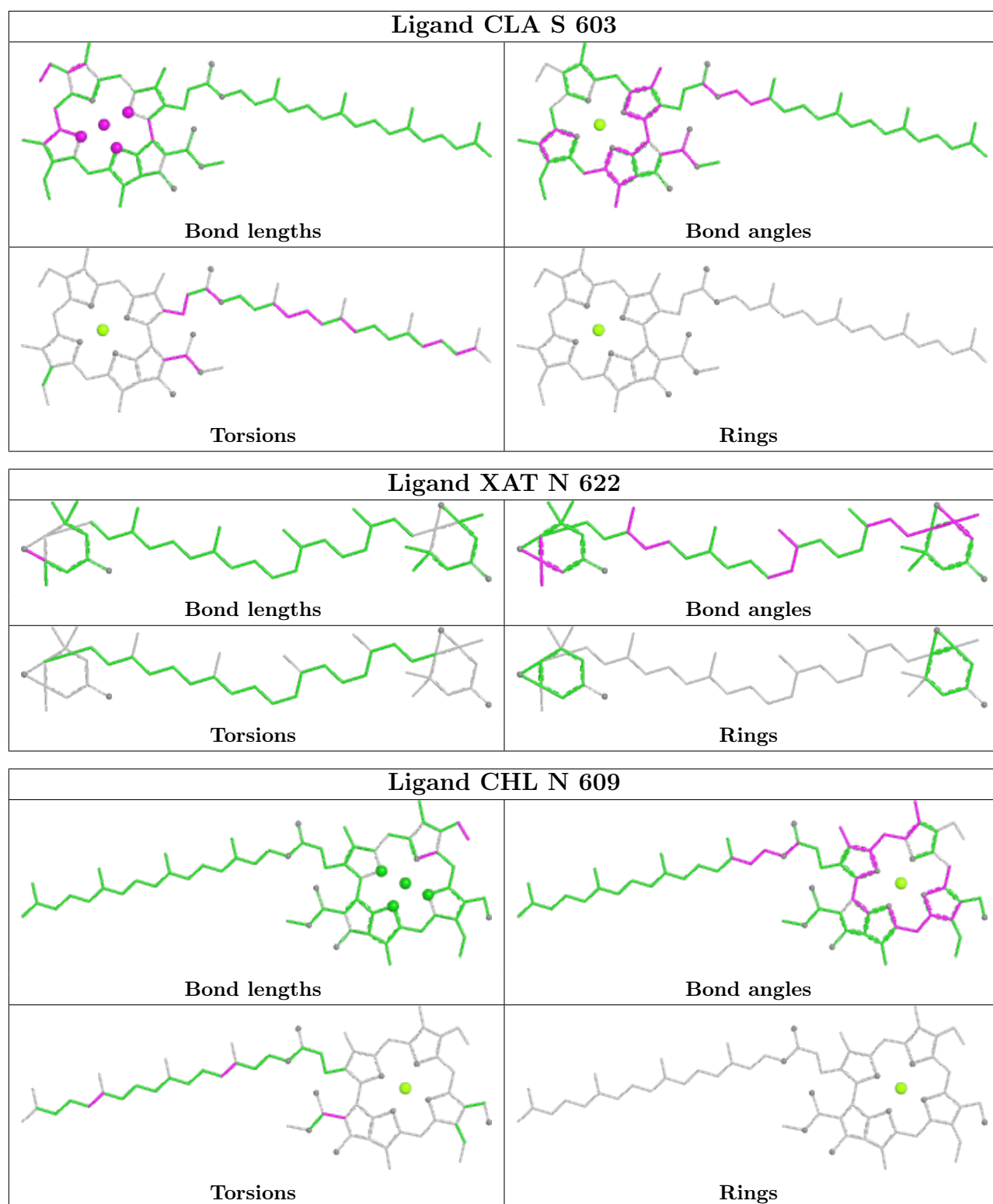


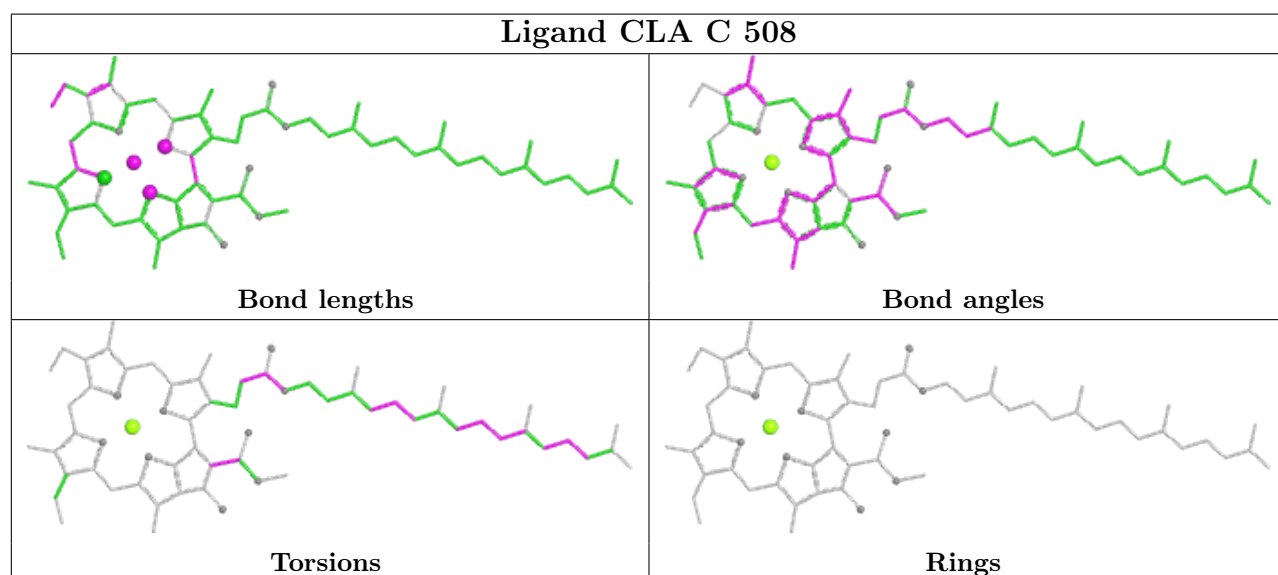
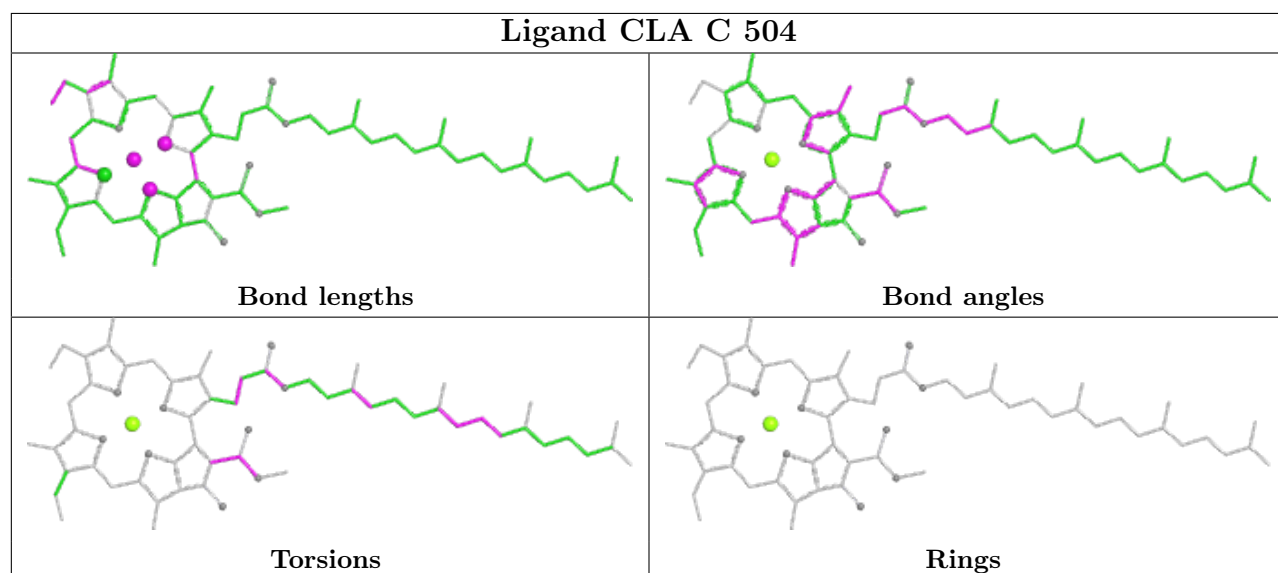
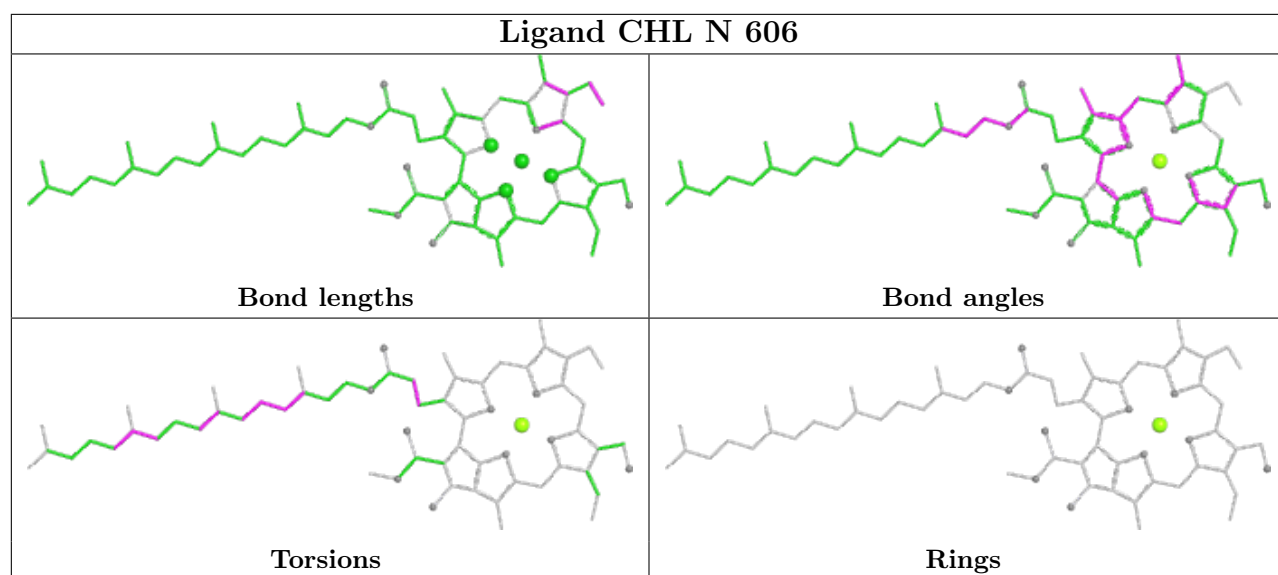


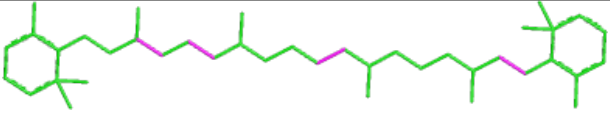
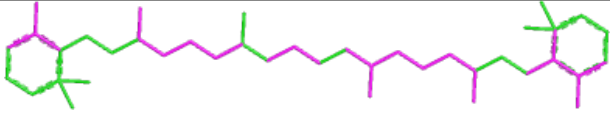
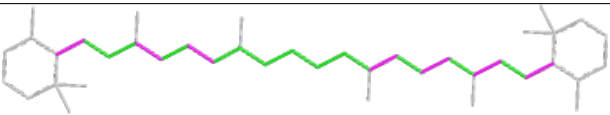
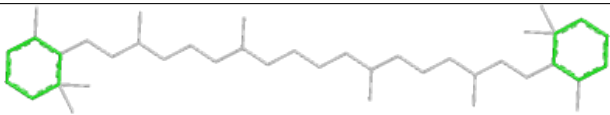
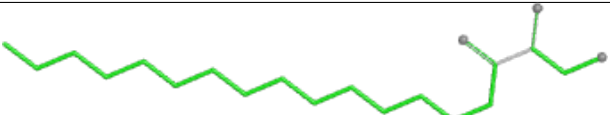
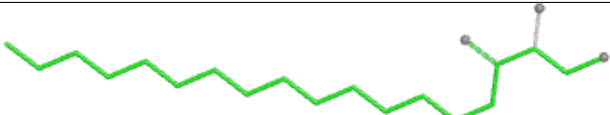
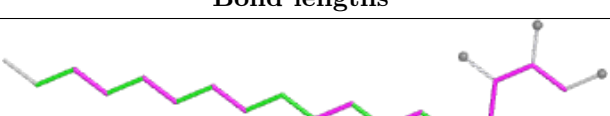
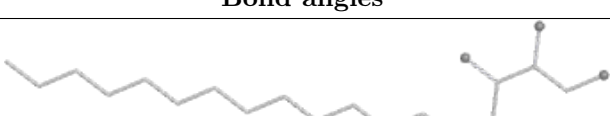
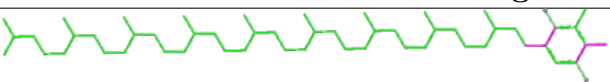
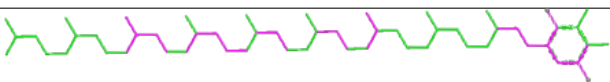
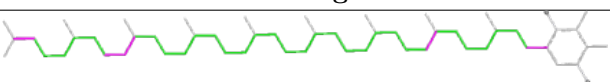
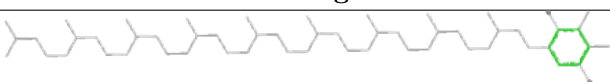
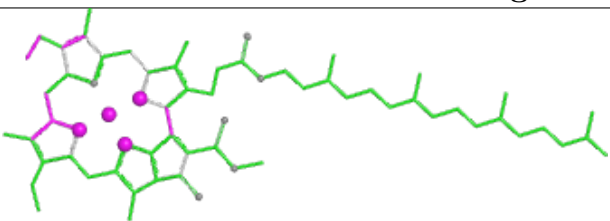
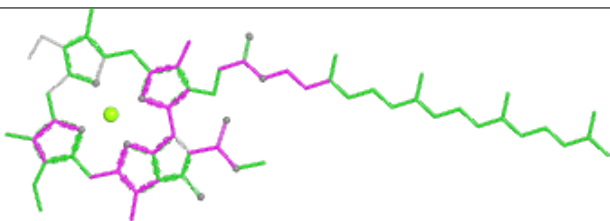
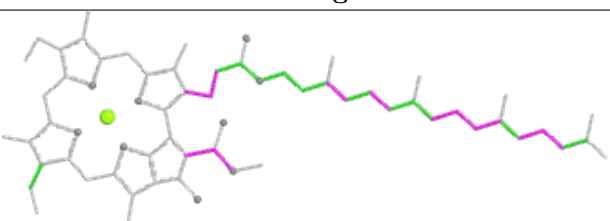
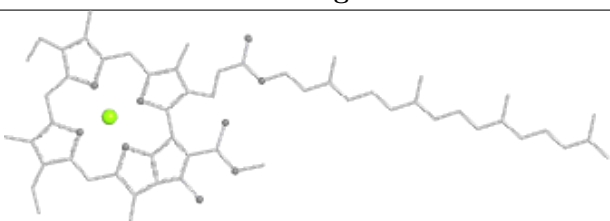


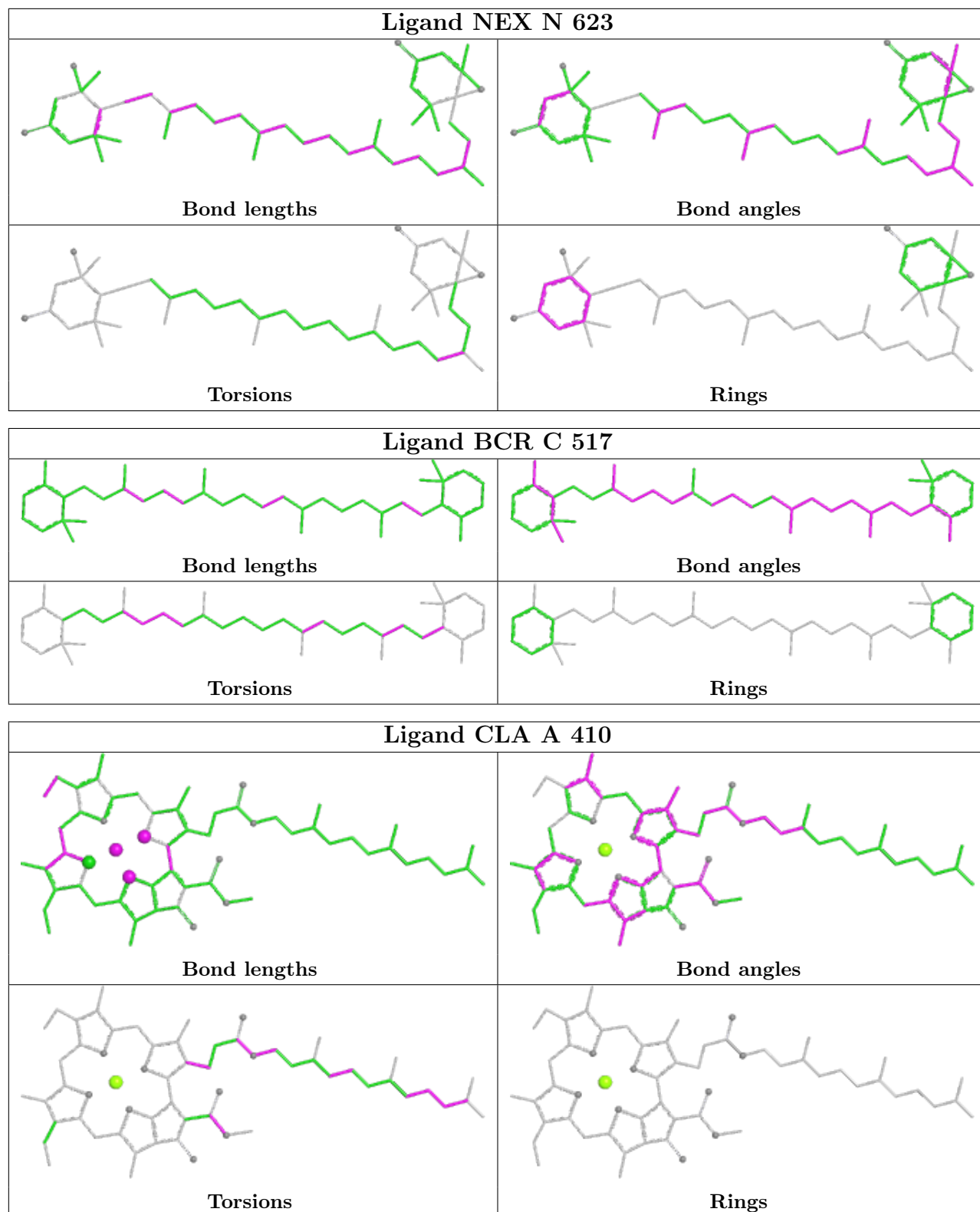


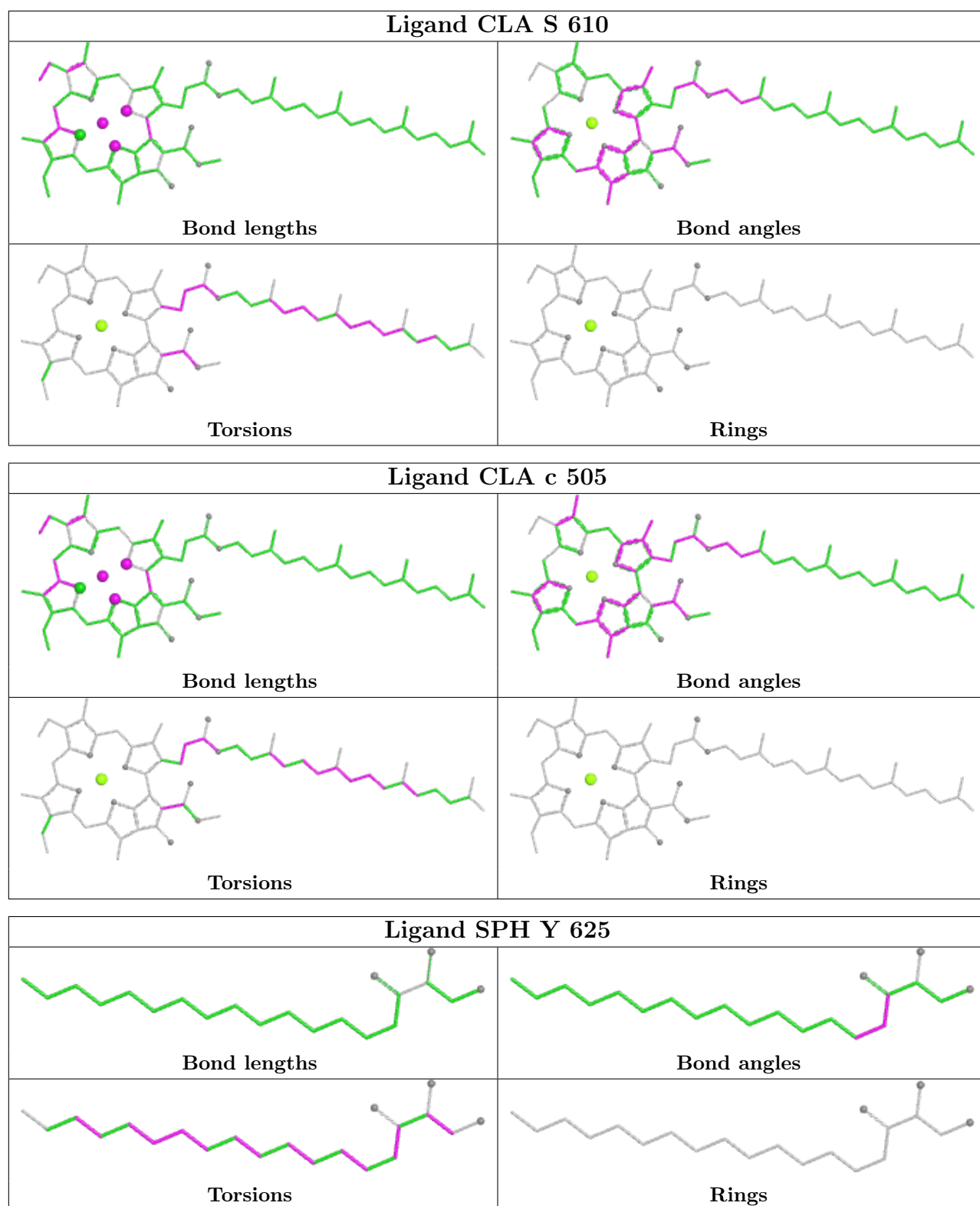


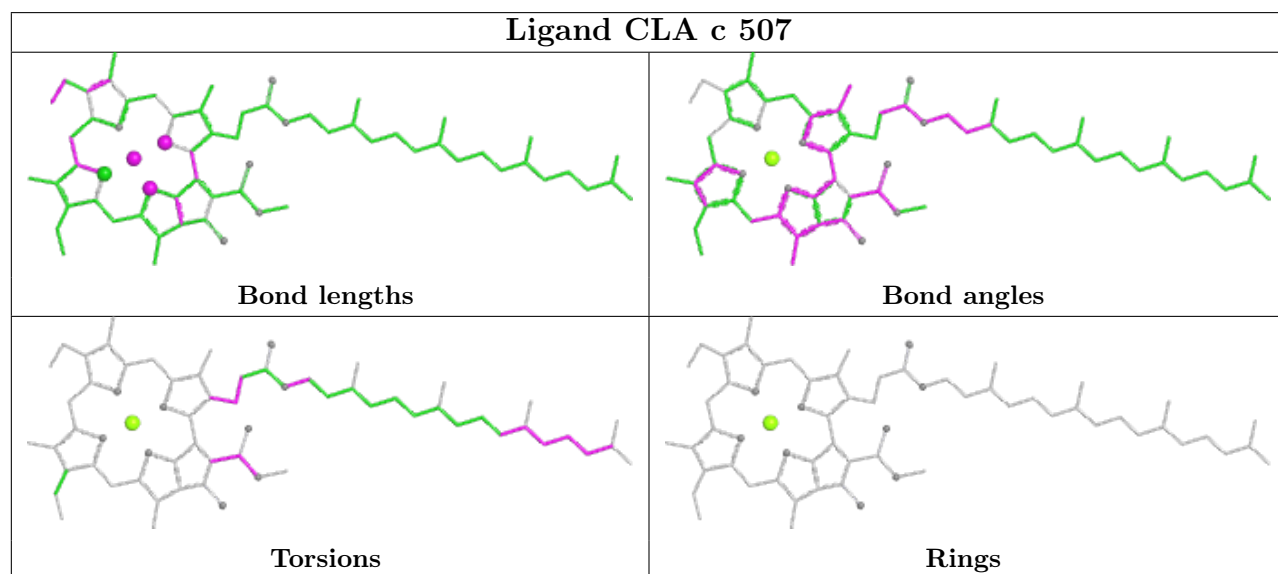
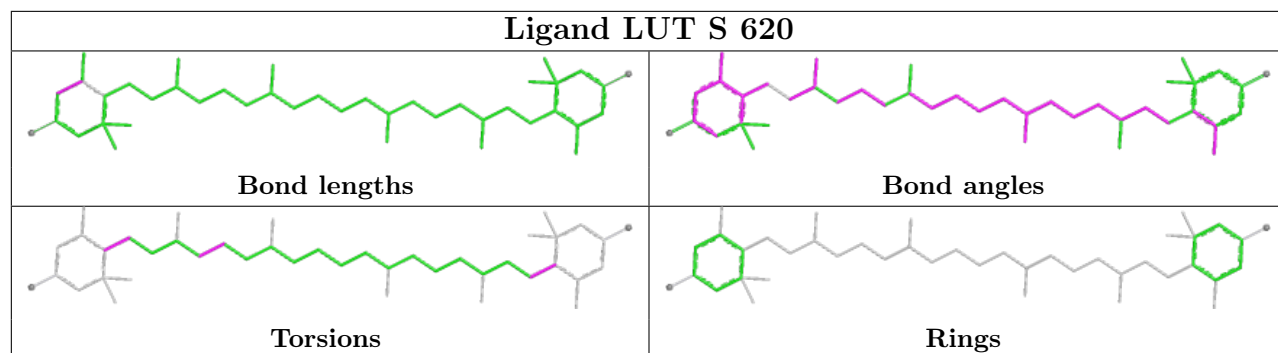


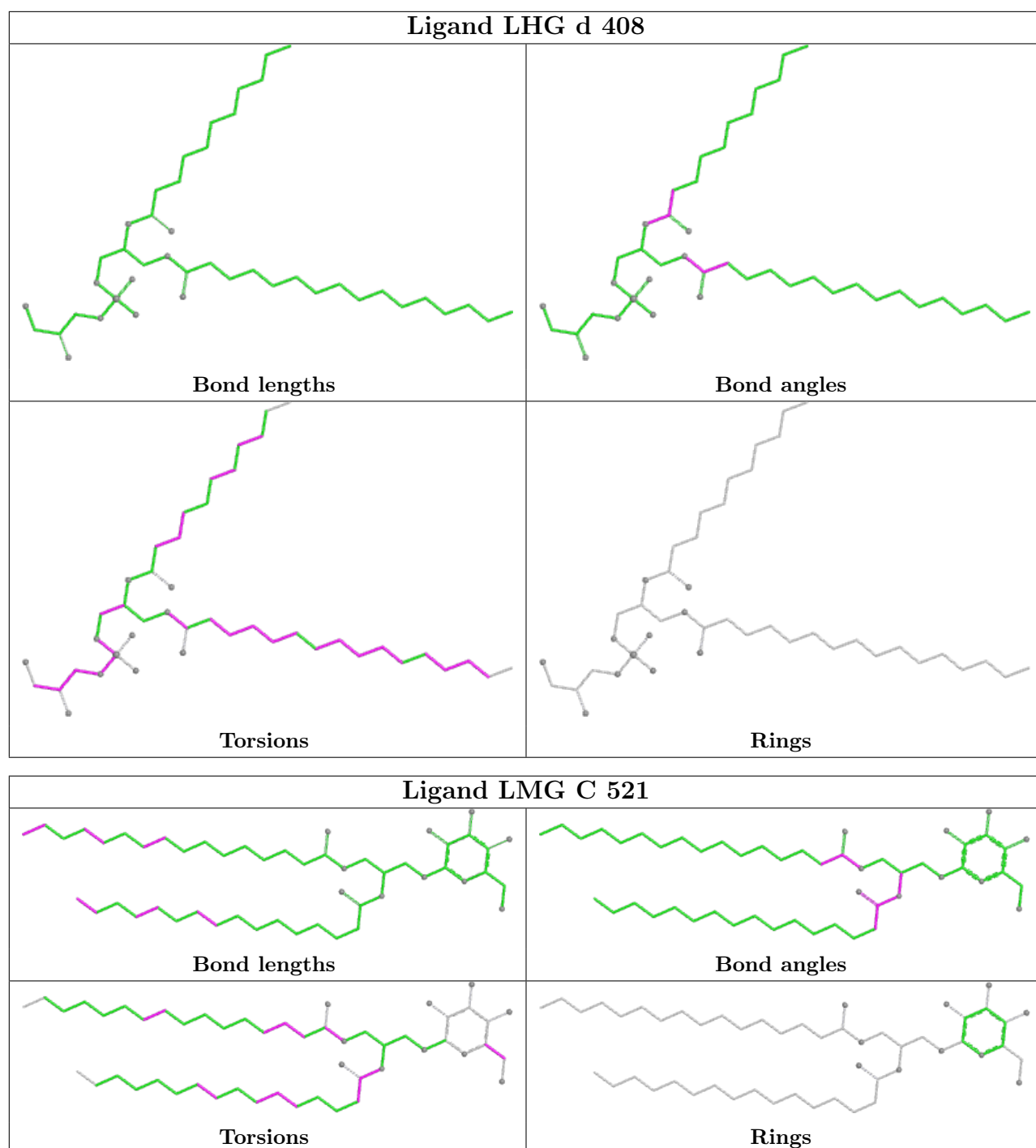


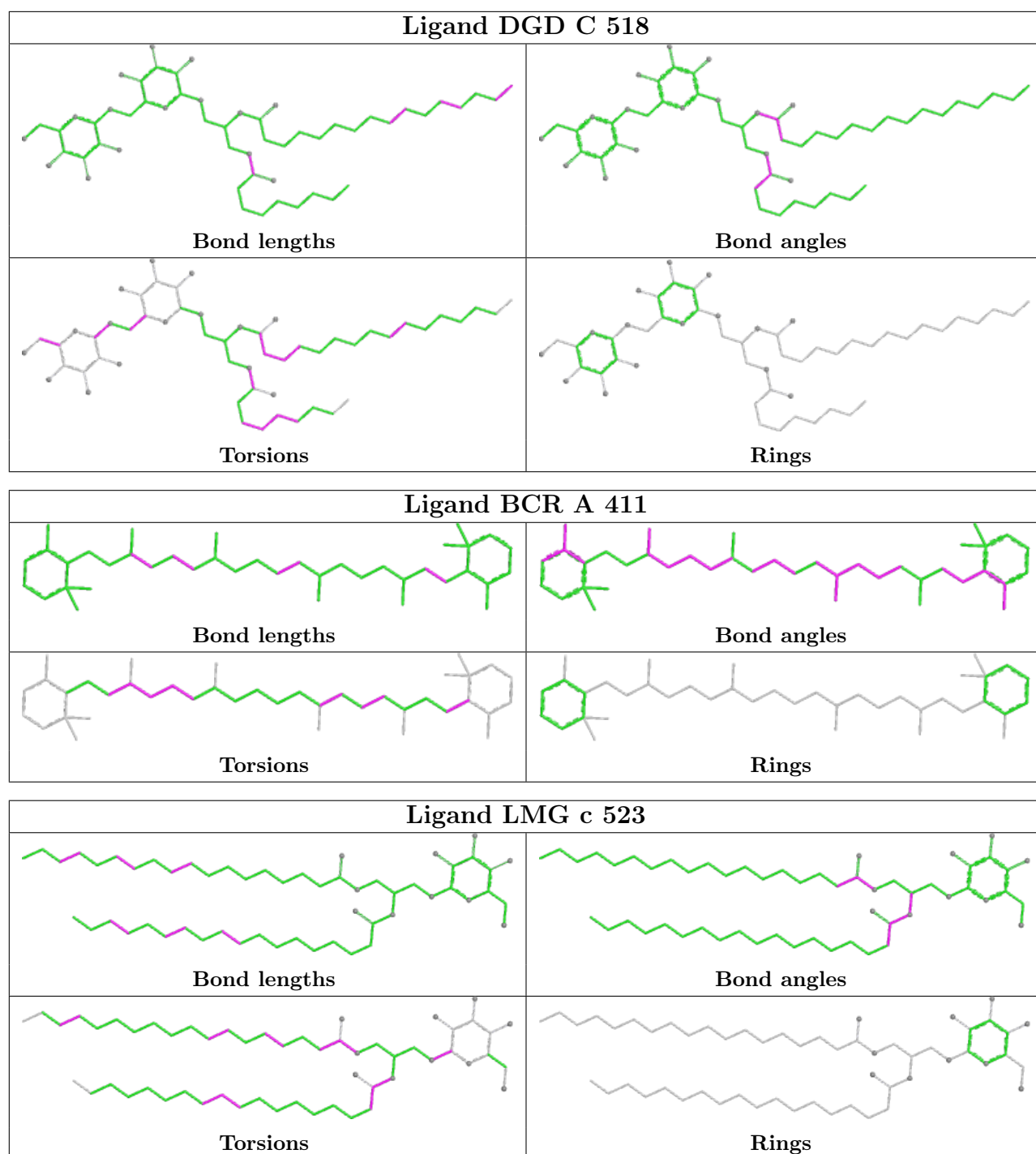
Ligand BCR D 404	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand SPH a 414	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 D 405	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA S 611	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

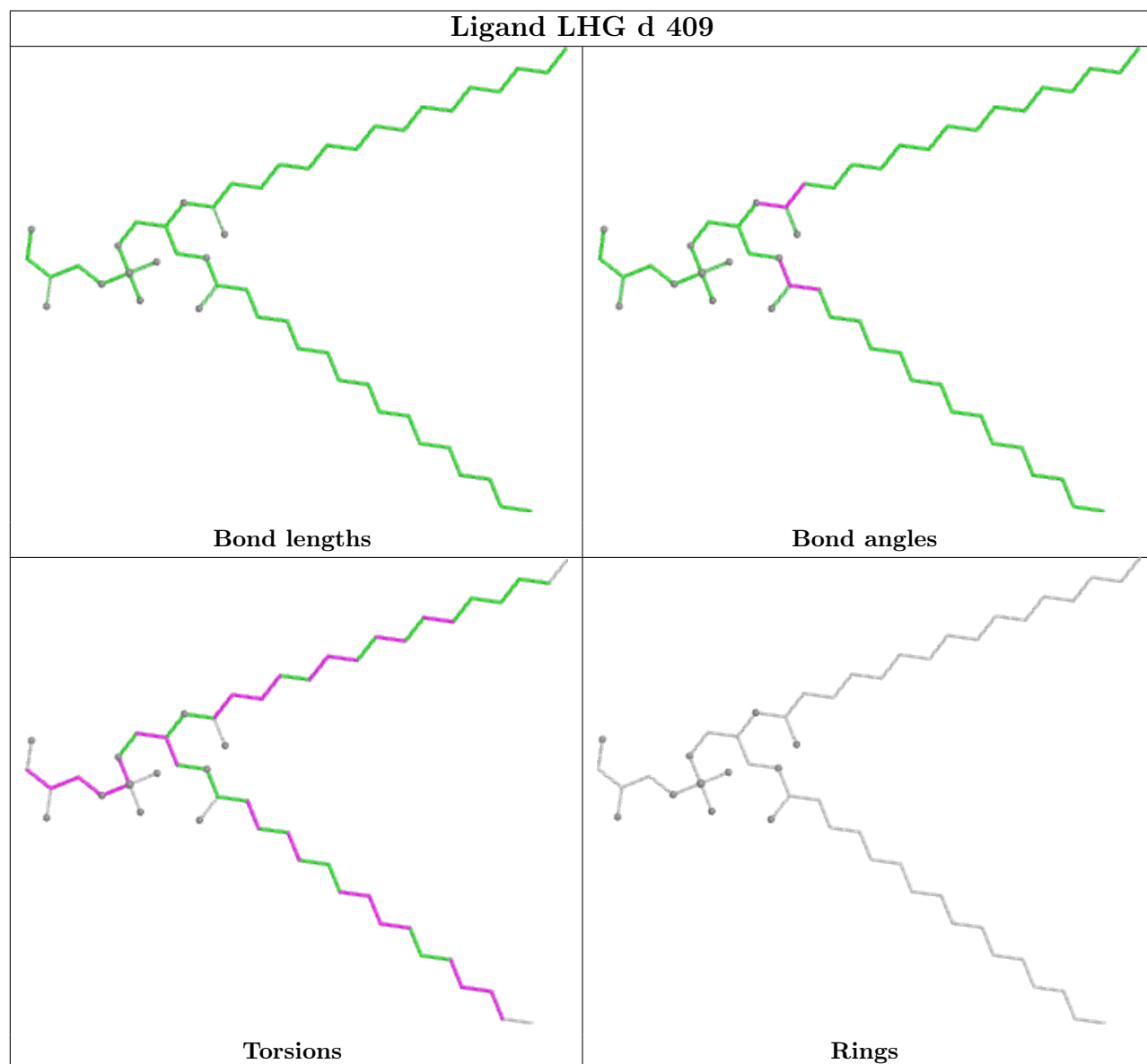
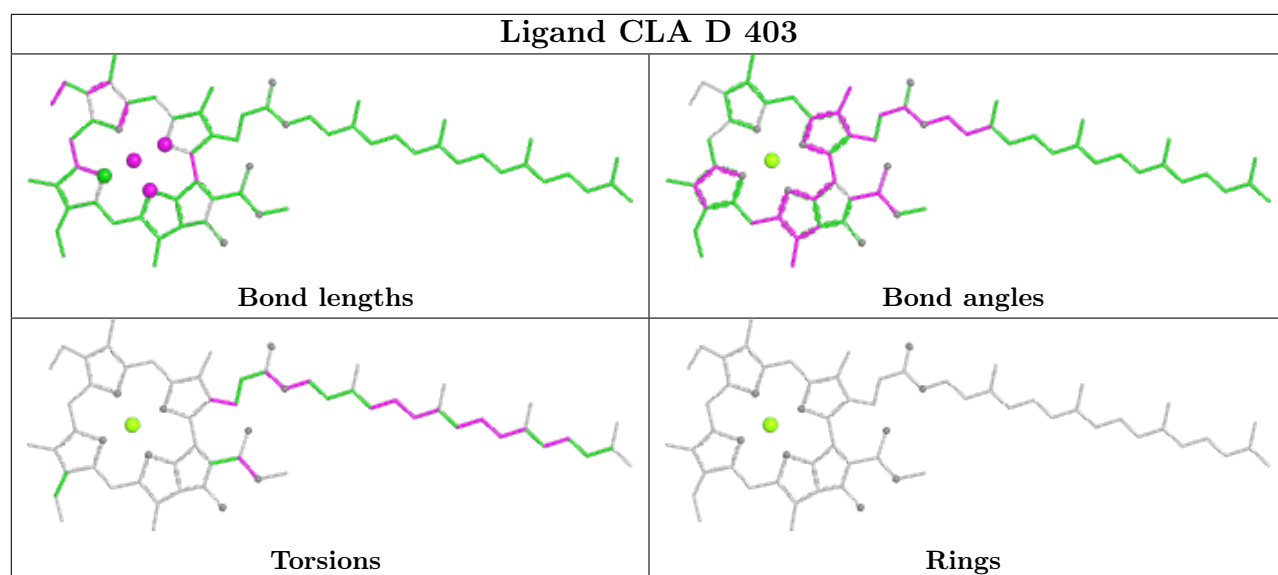


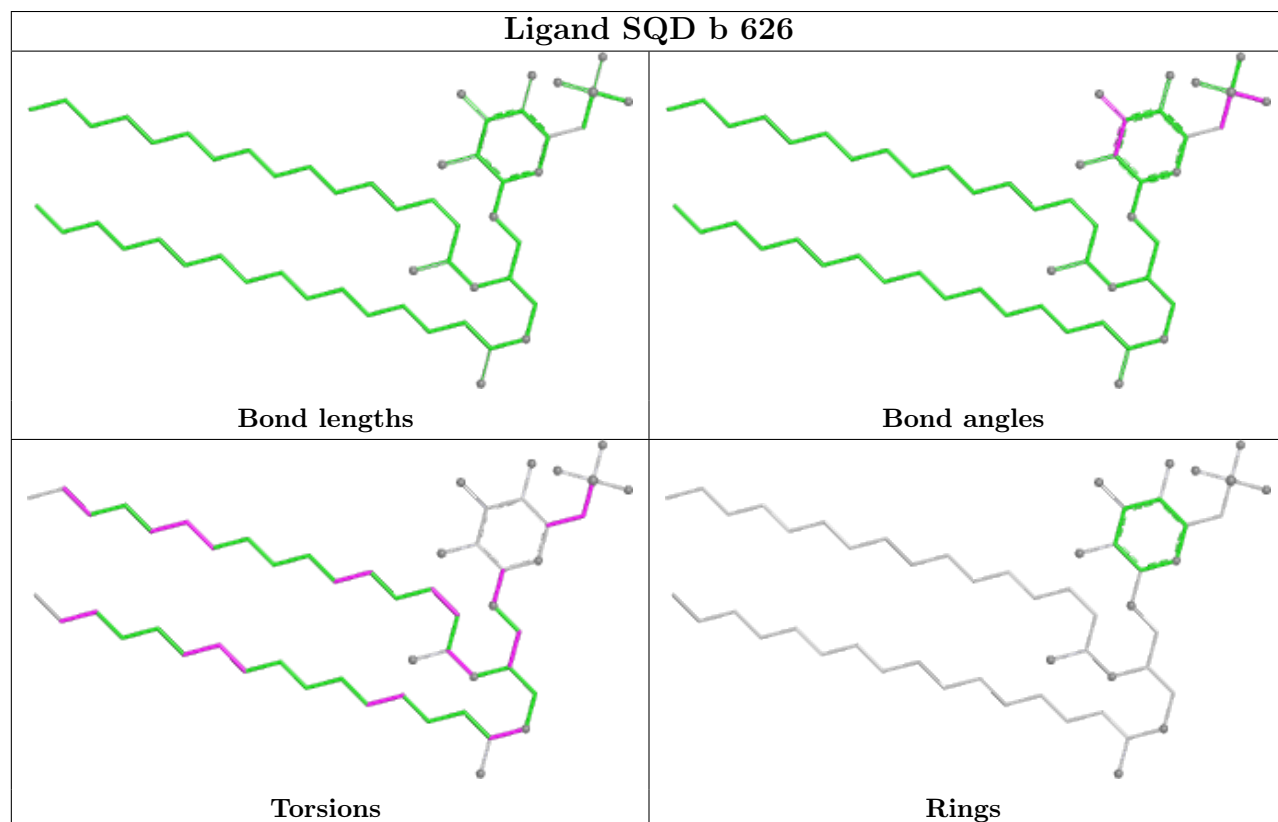
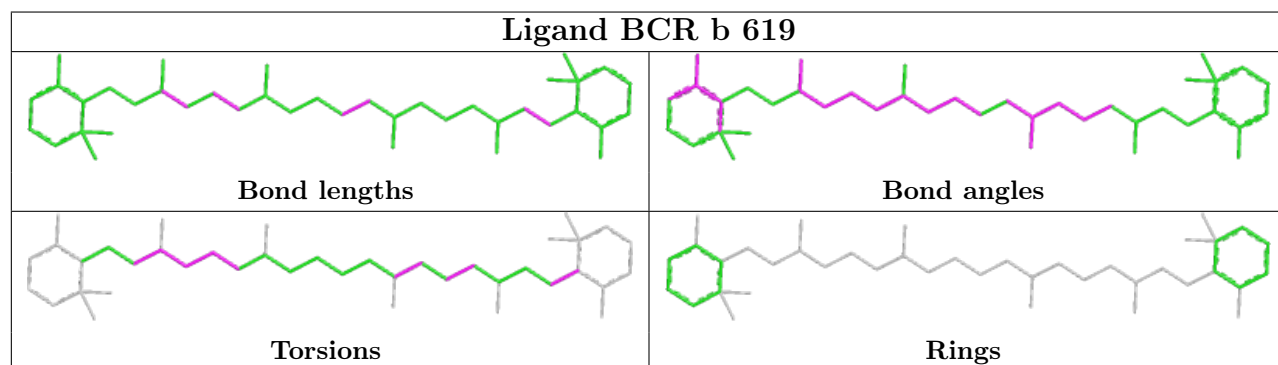
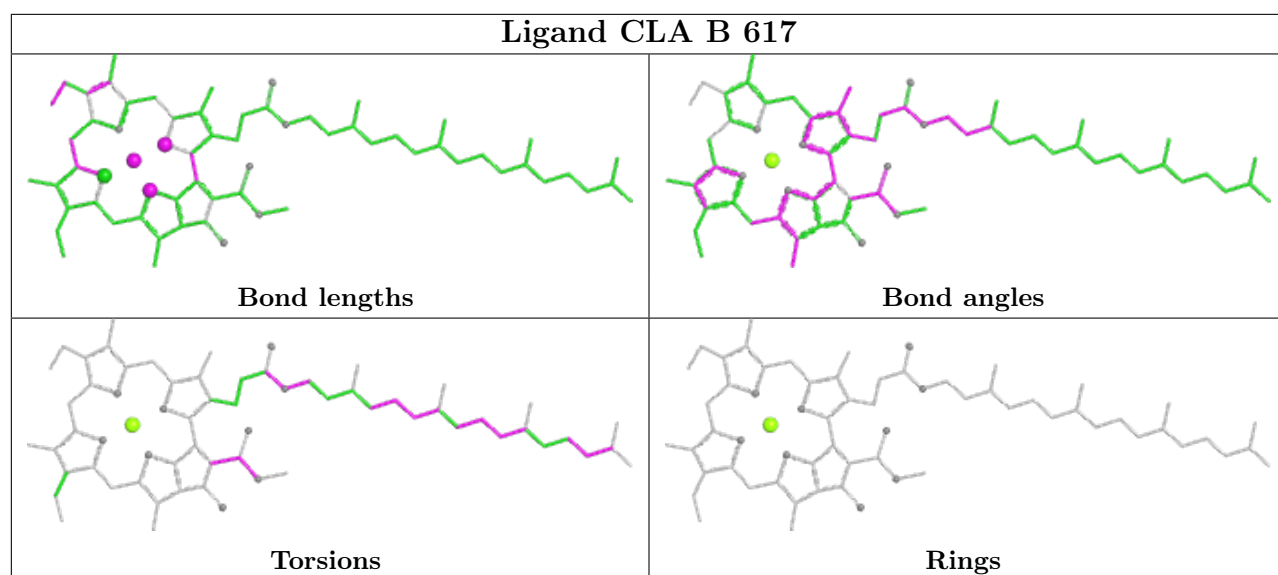


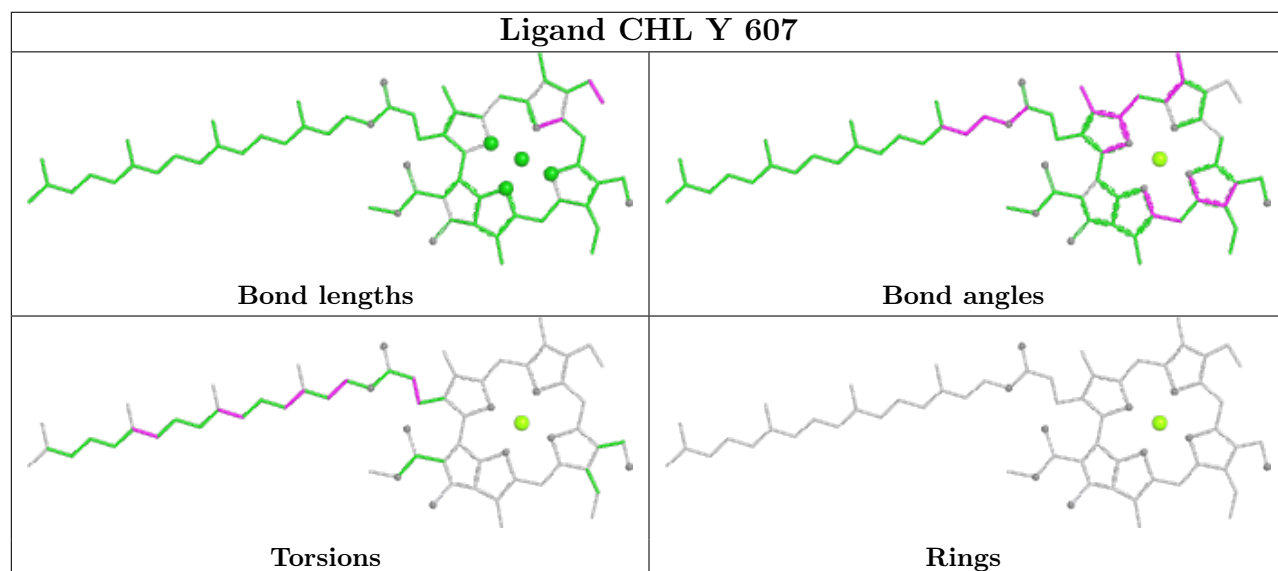
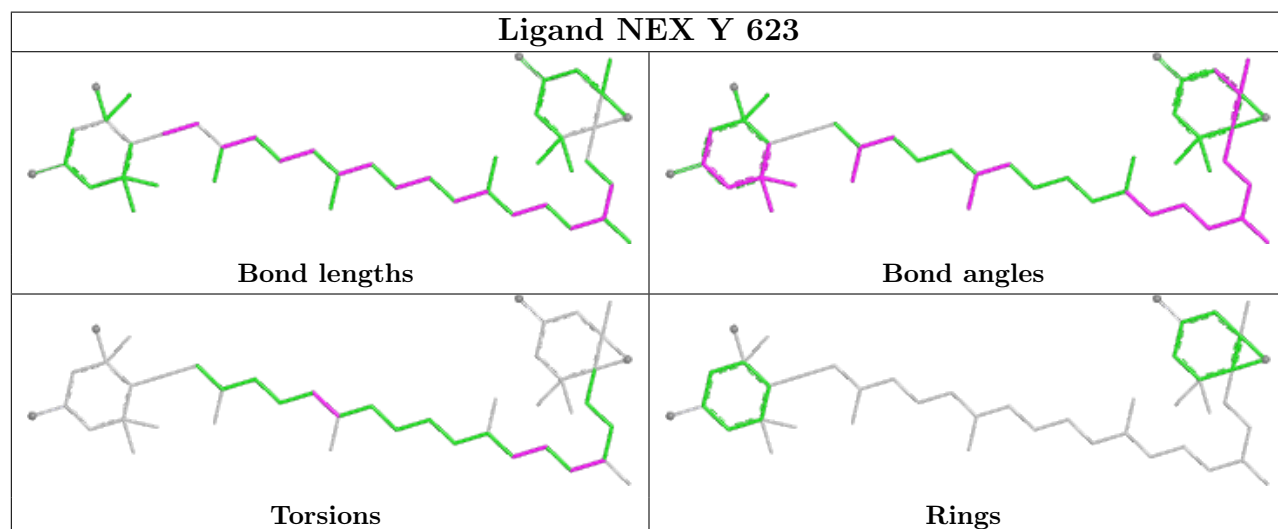
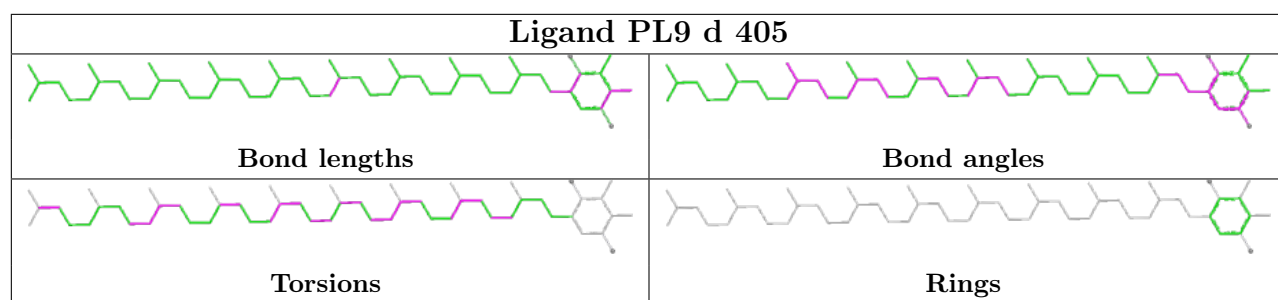


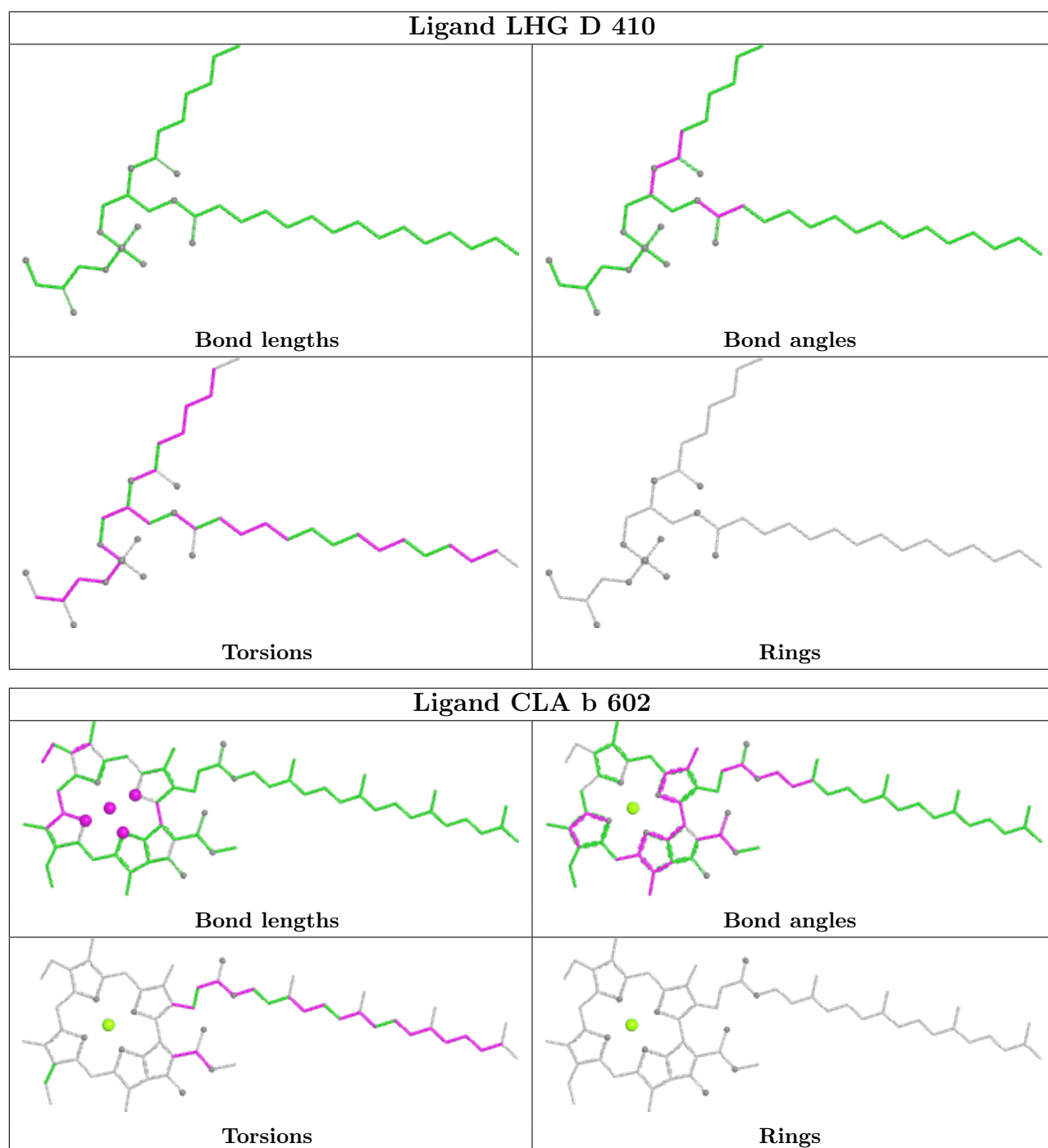


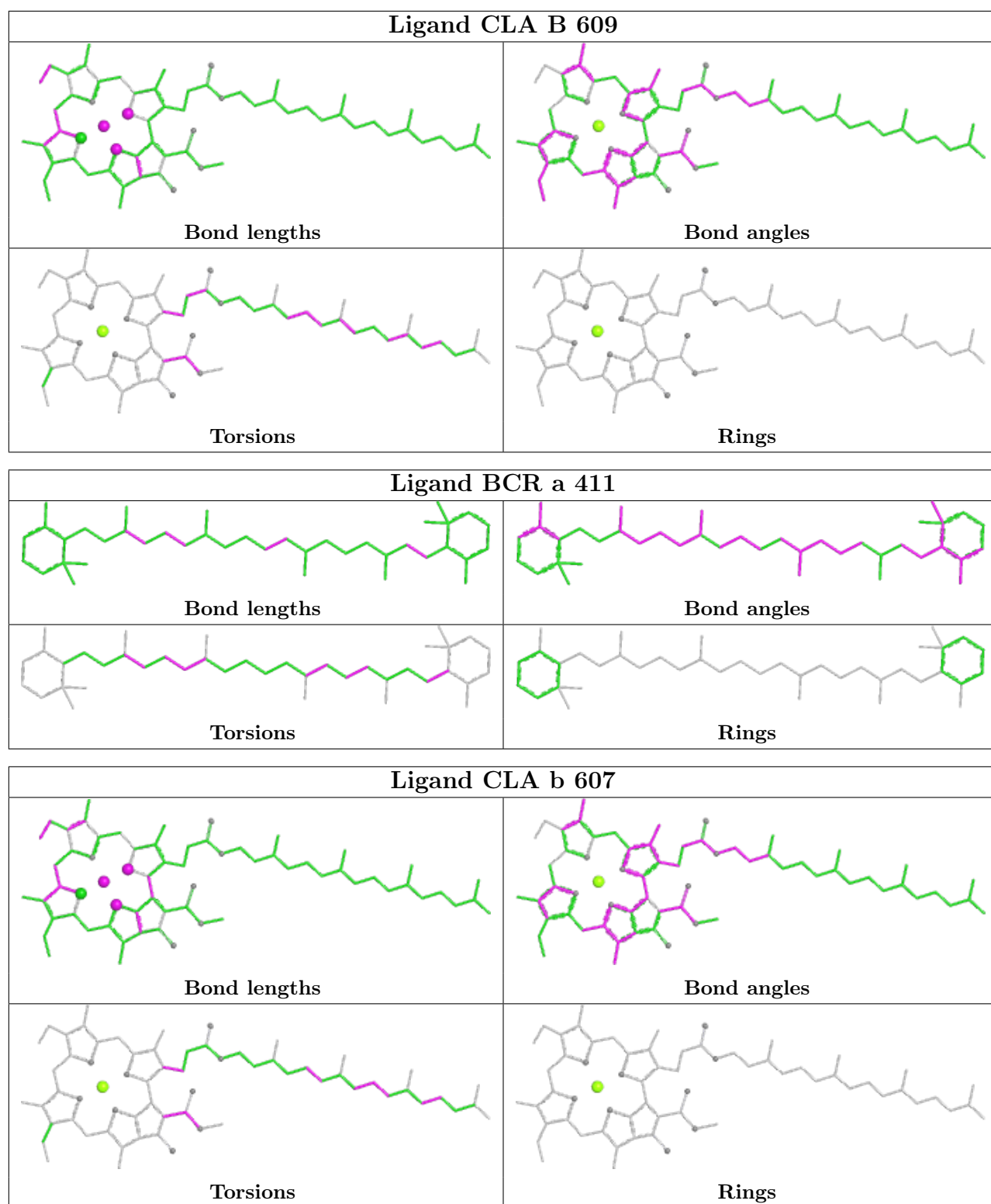


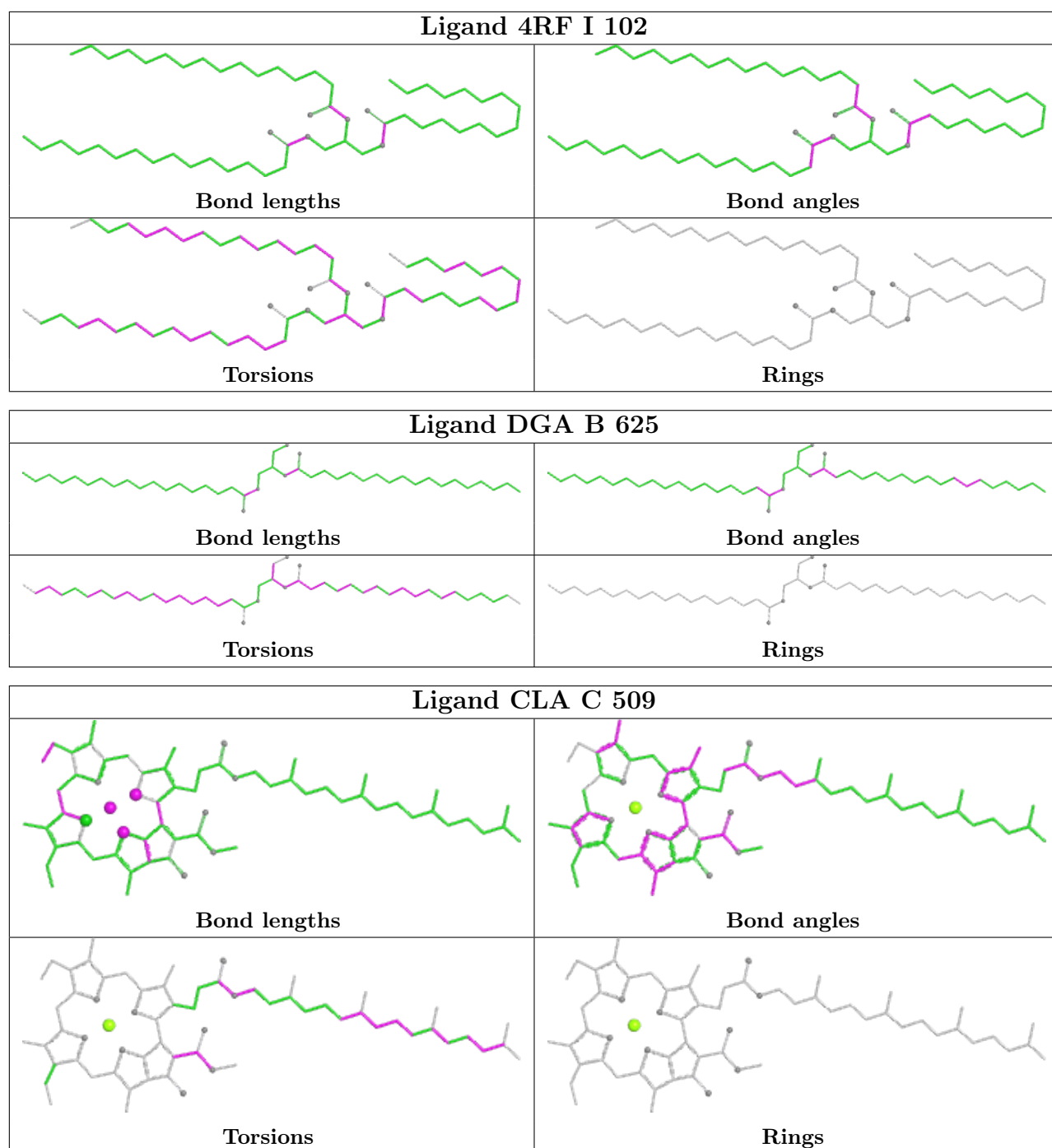


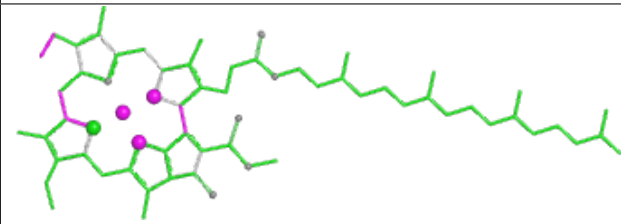
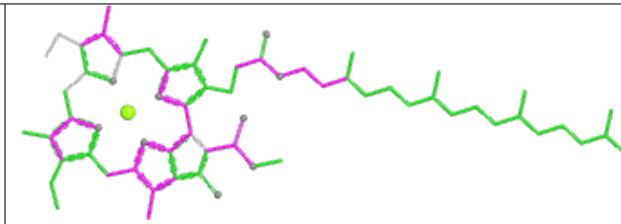
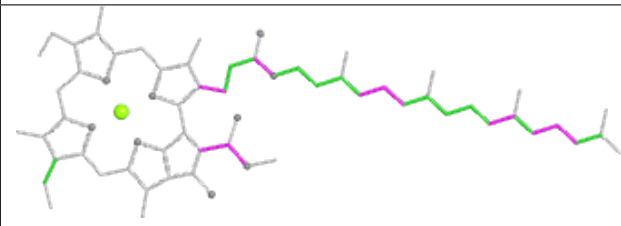
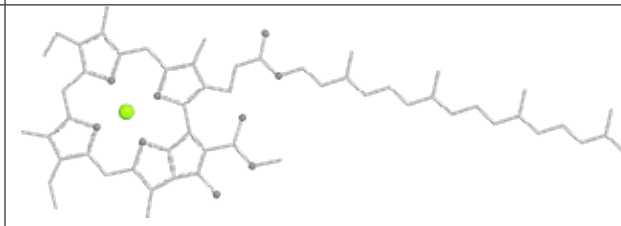


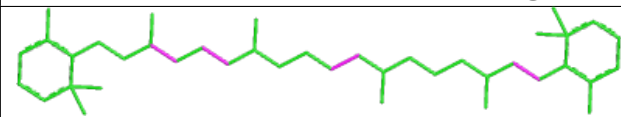
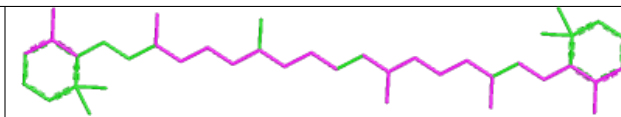
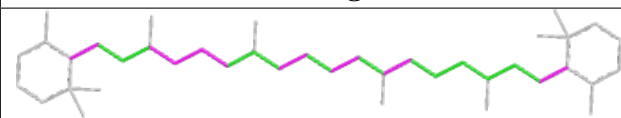
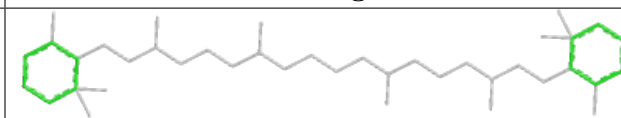


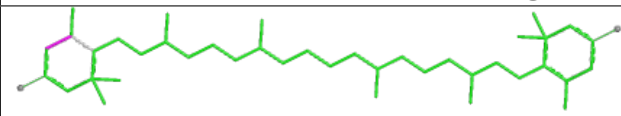
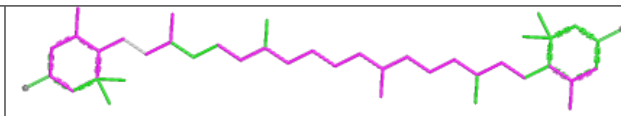
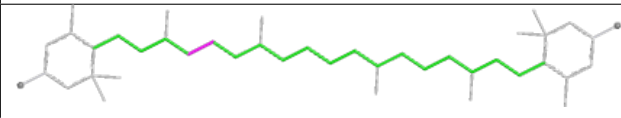
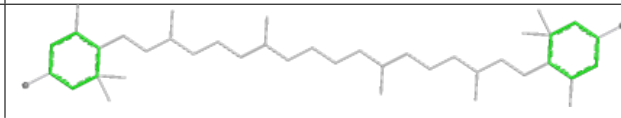


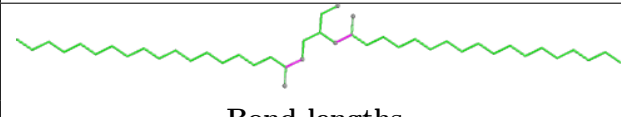
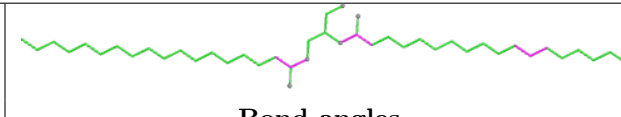
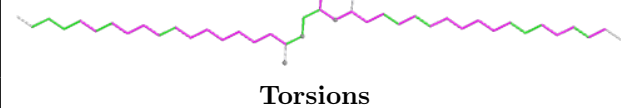
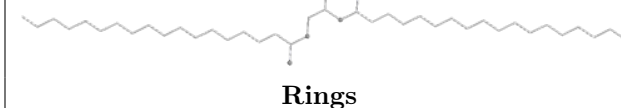


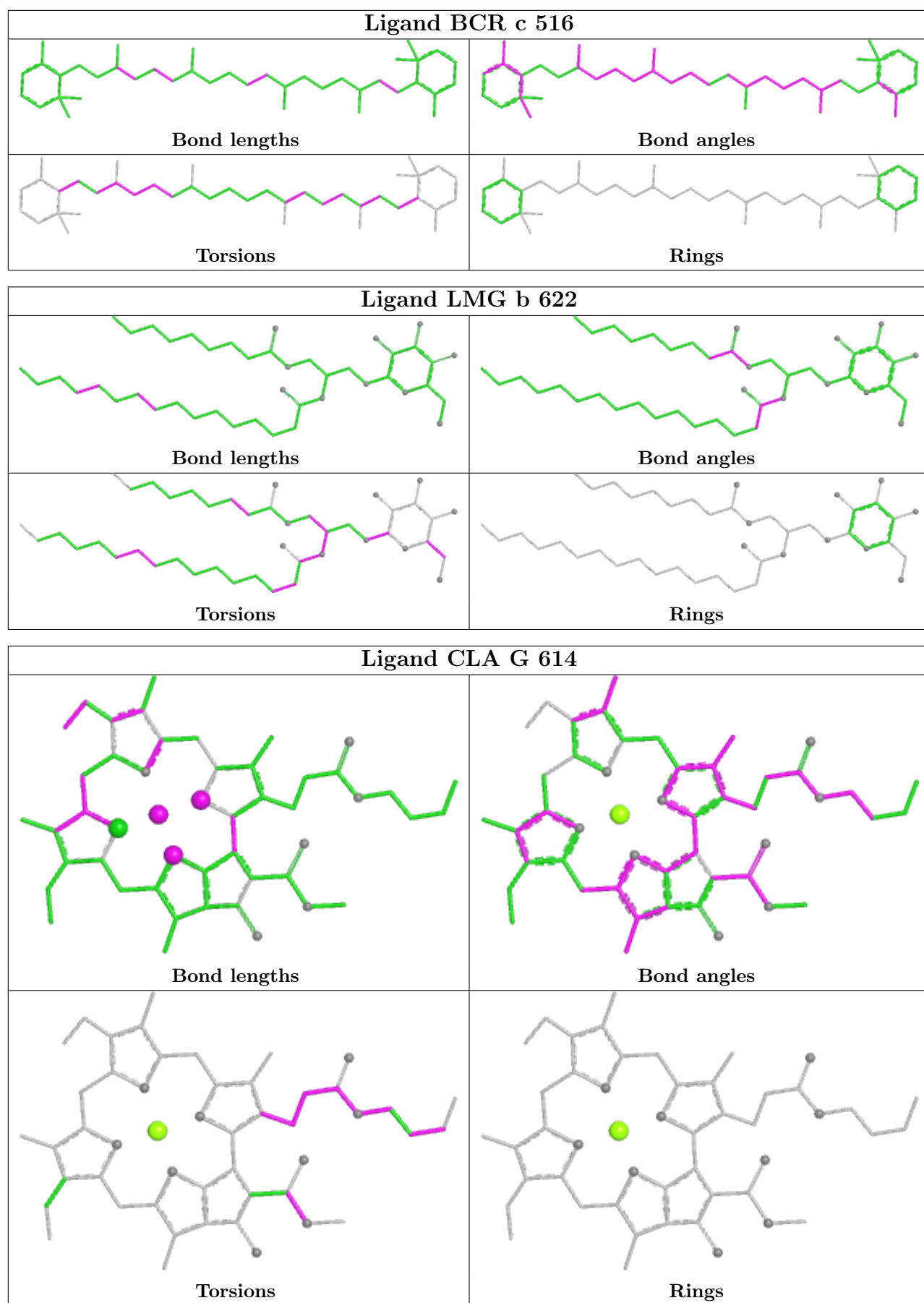


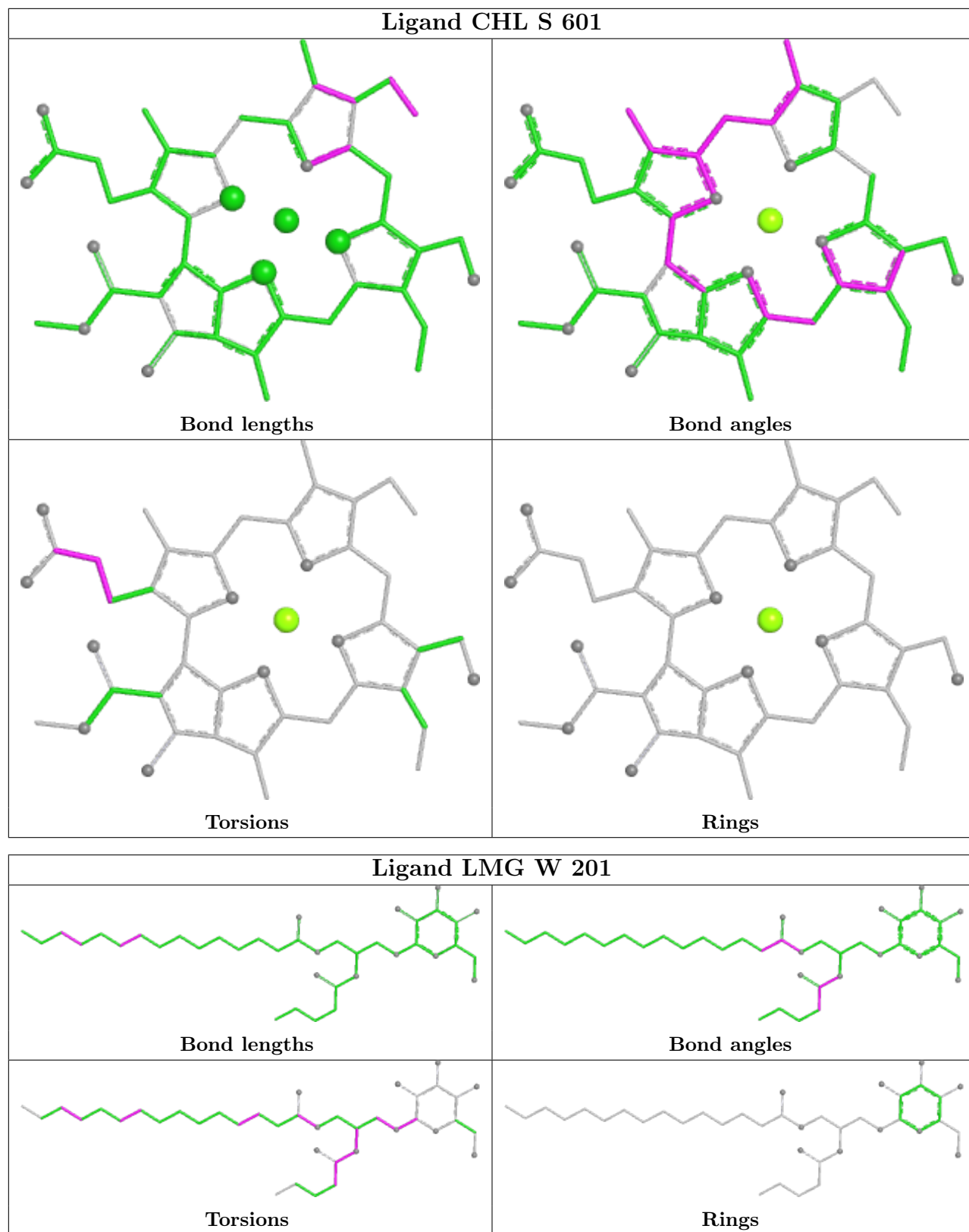
Ligand CLA b 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

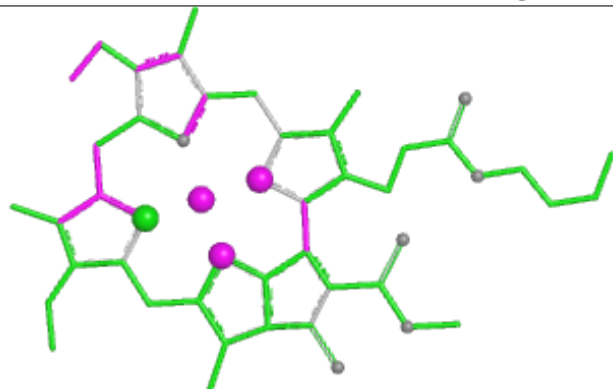
Ligand LUT S 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGA b 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

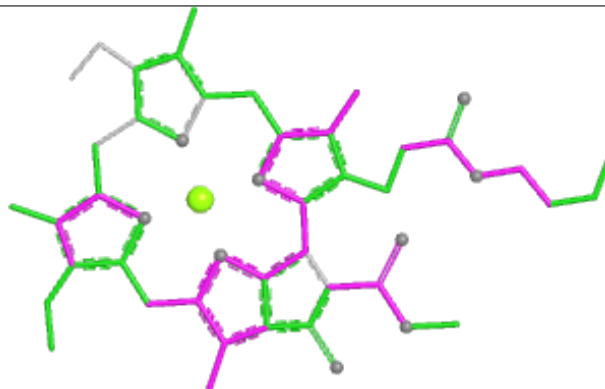




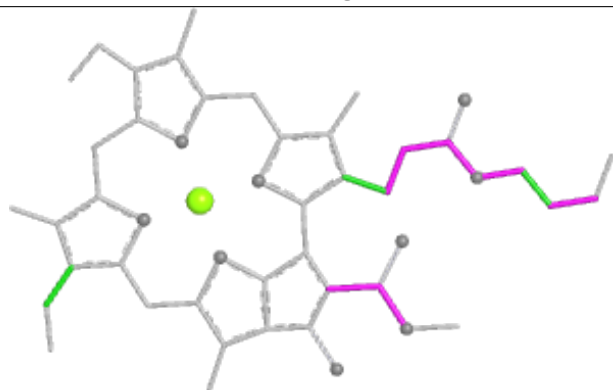
Ligand CLA N 611



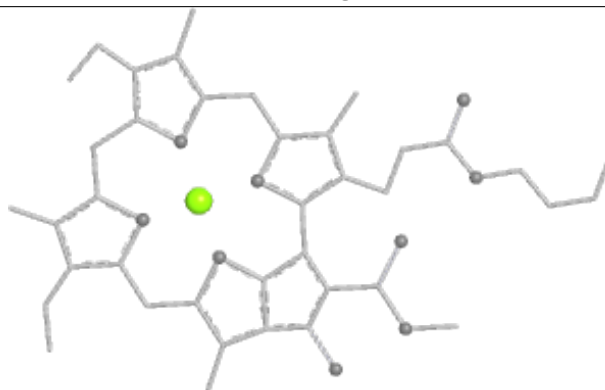
Bond lengths



Bond angles

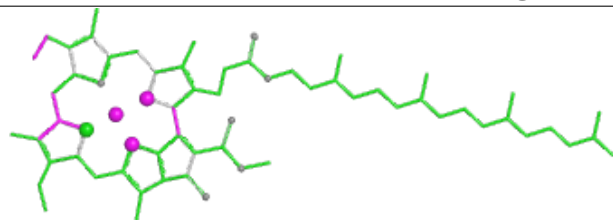


Torsions

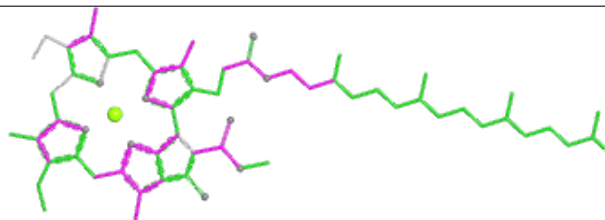


Rings

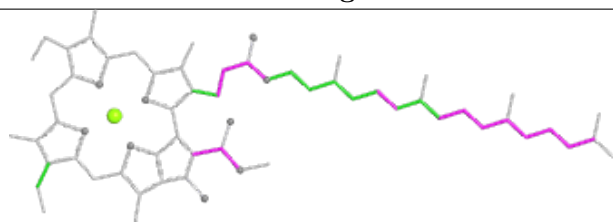
Ligand CLA Y 613



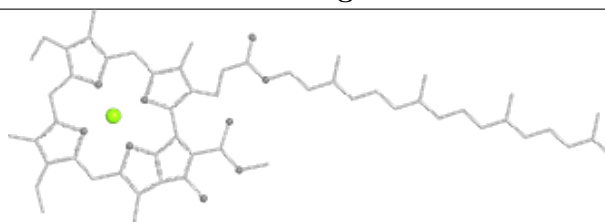
Bond lengths



Bond angles

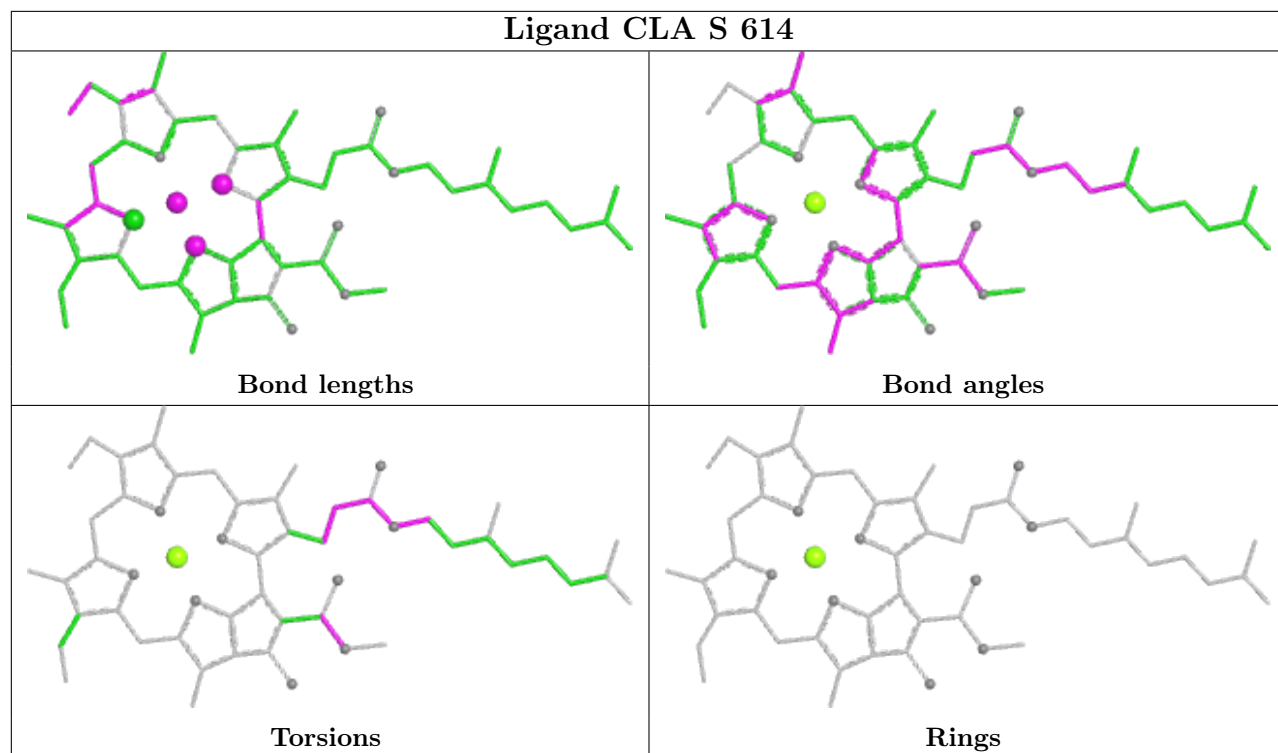


Torsions

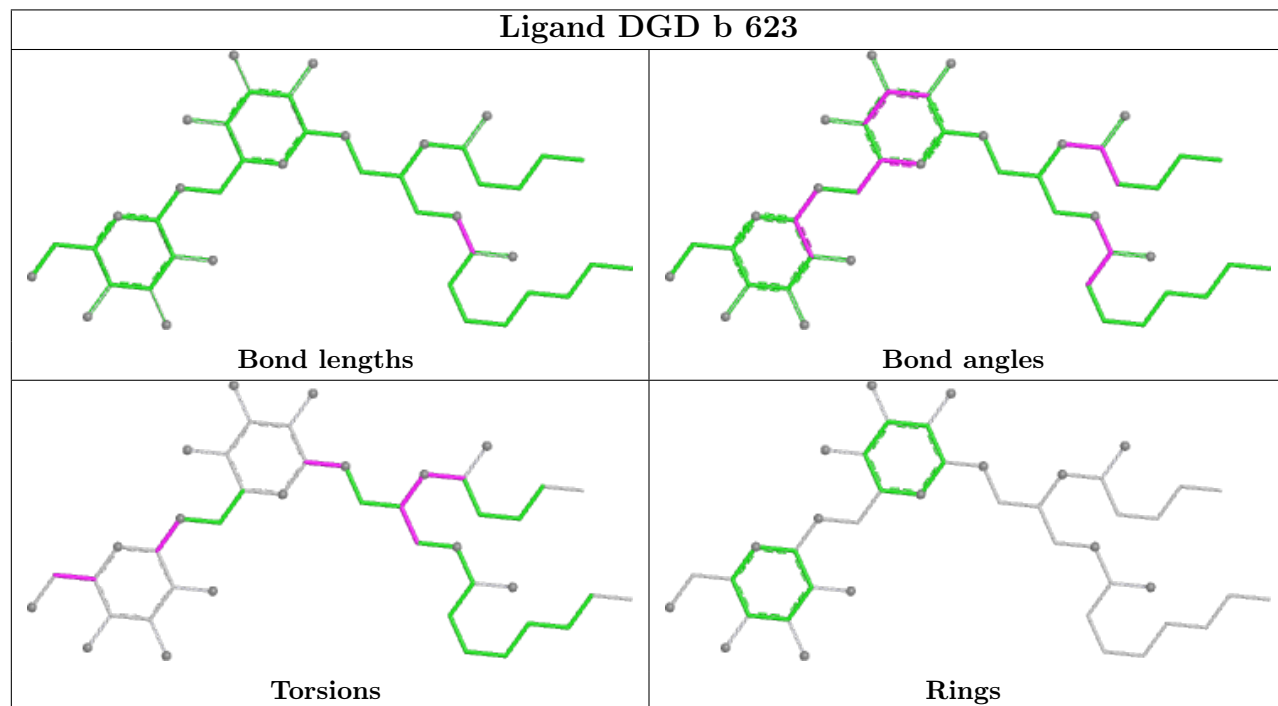


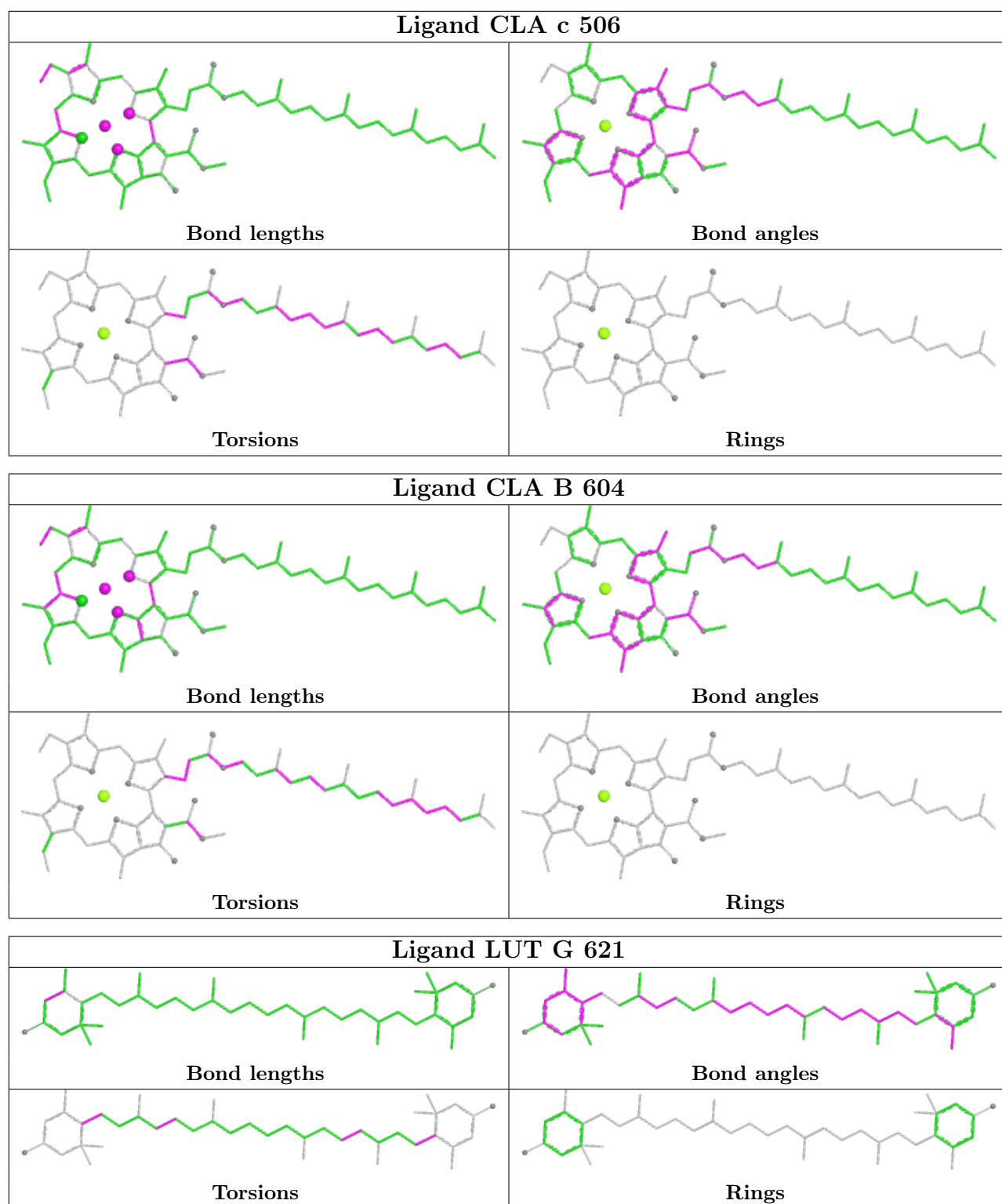
Rings

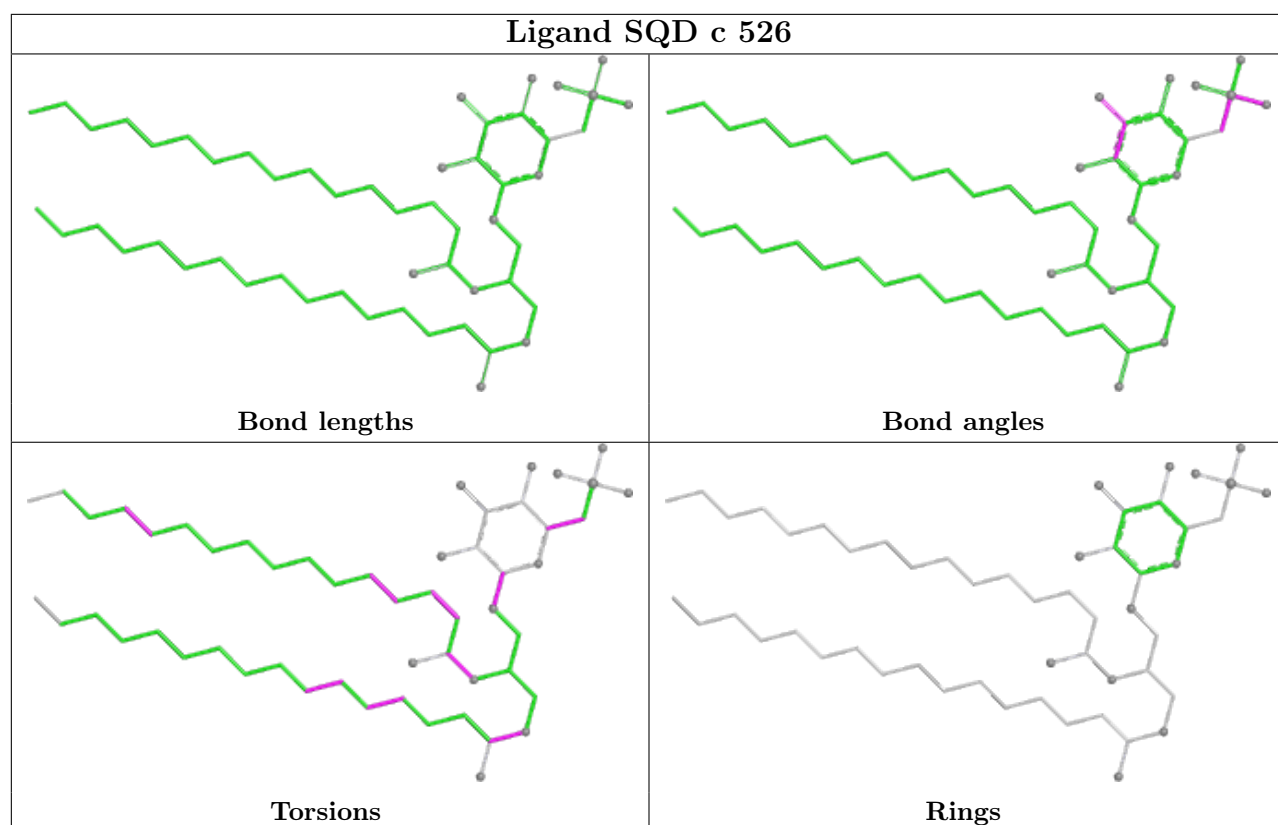
Ligand CLA S 614

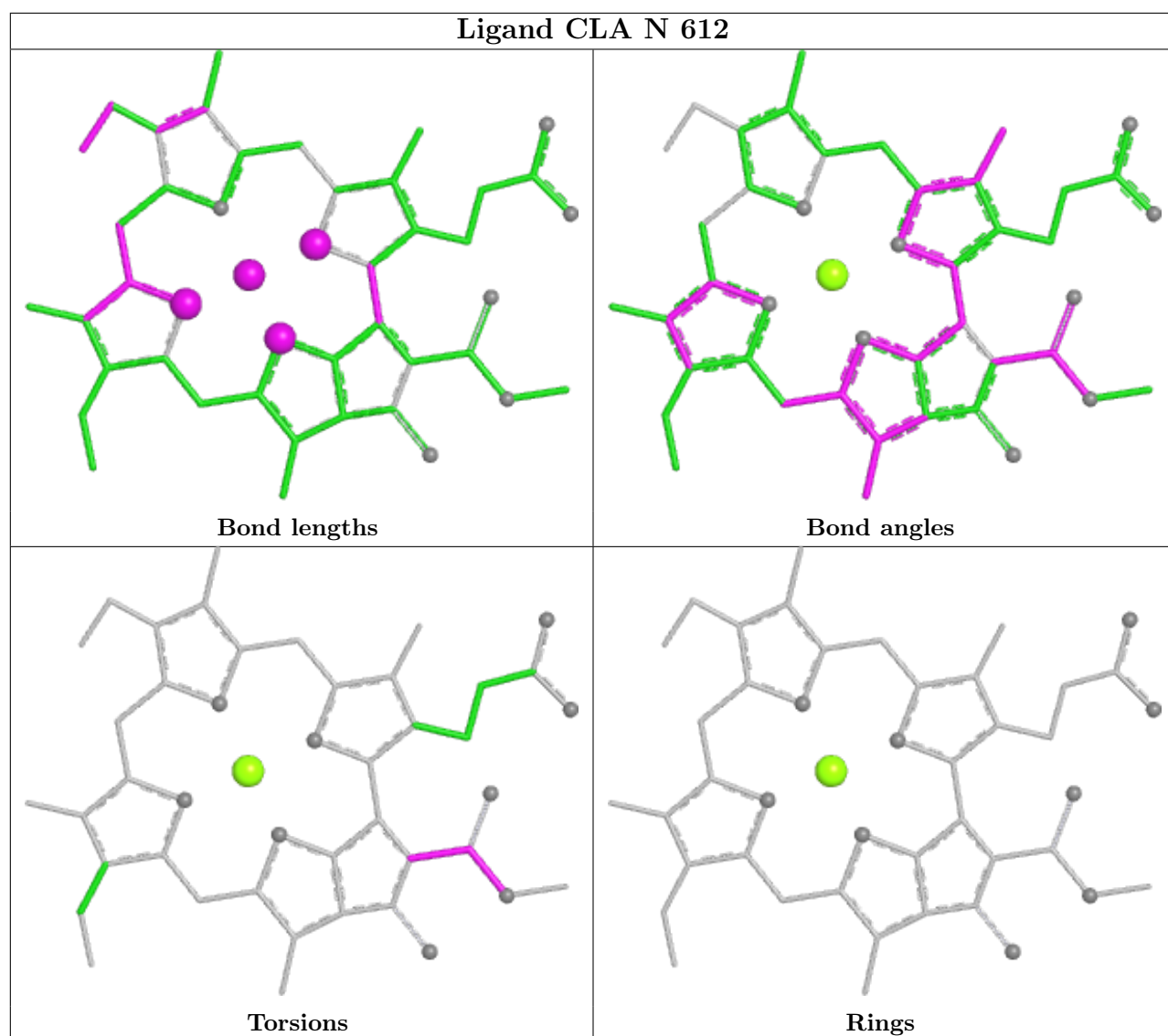


Ligand DGD b 623

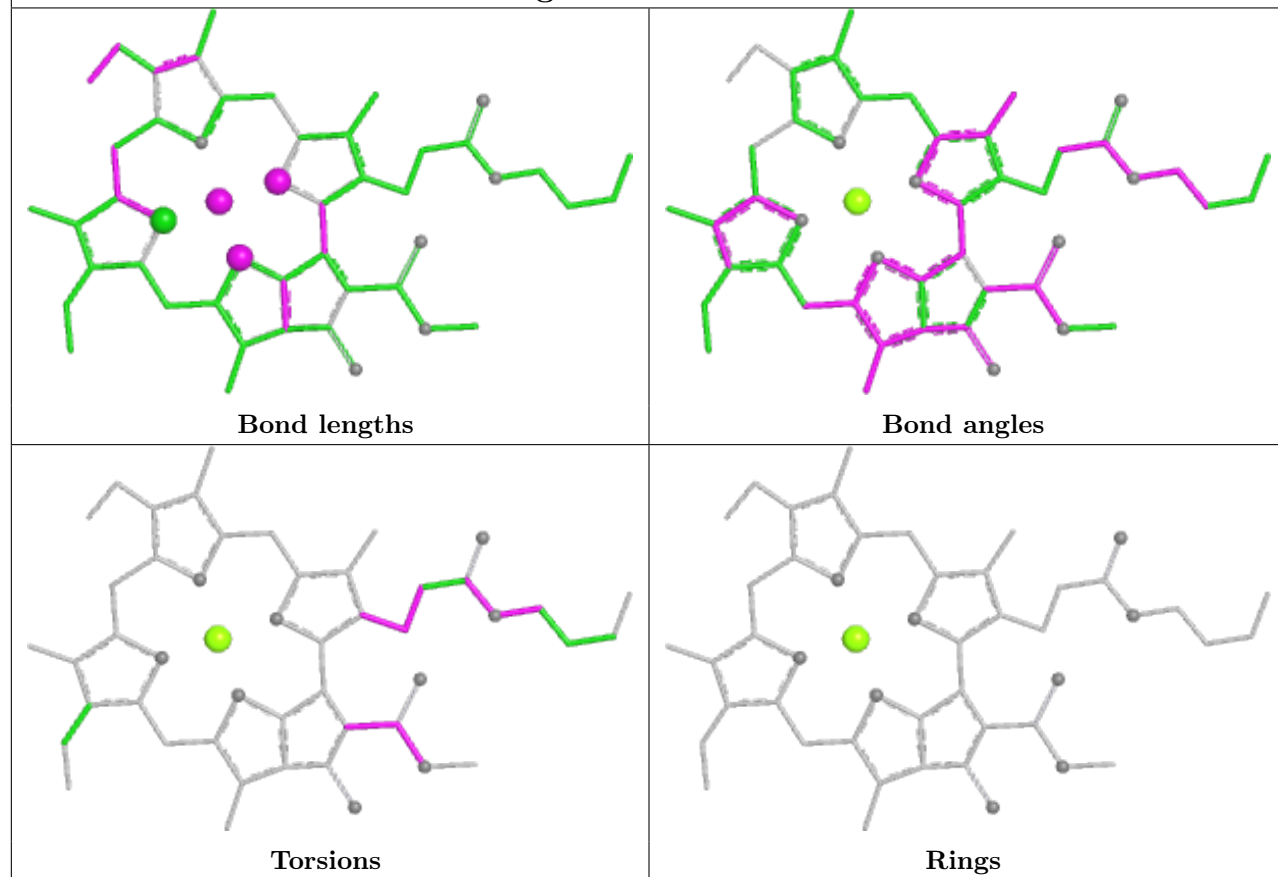




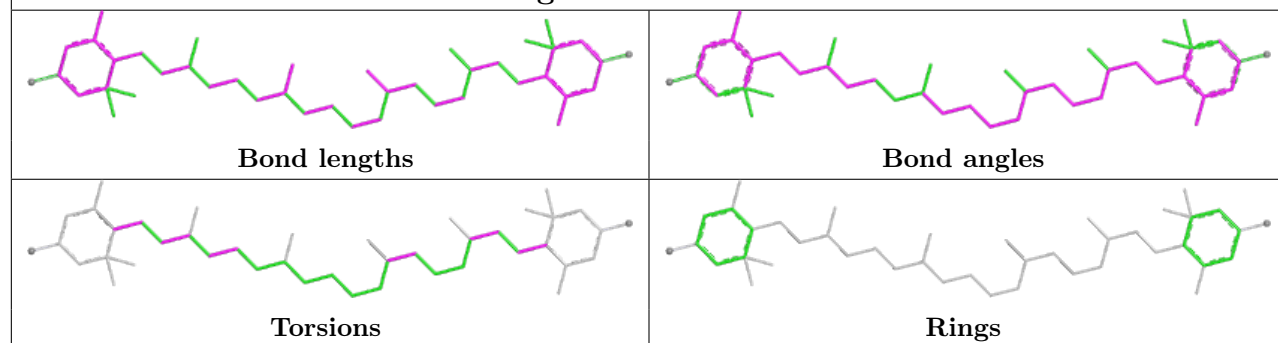




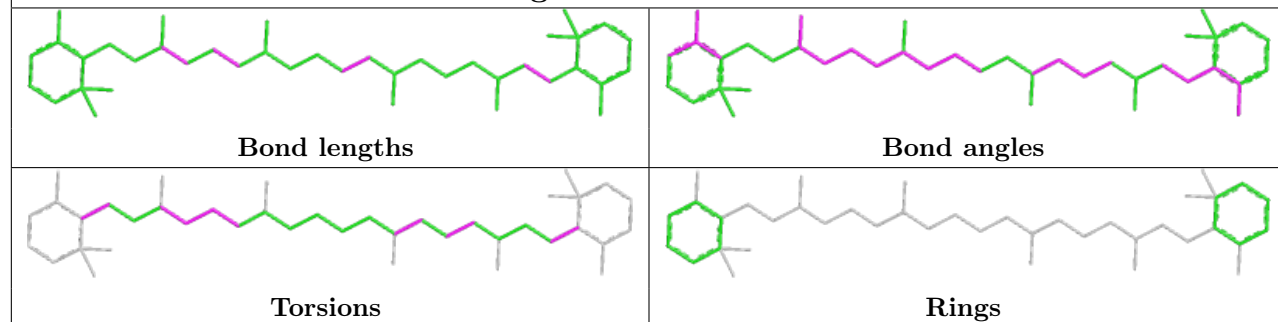
Ligand CLA a 407

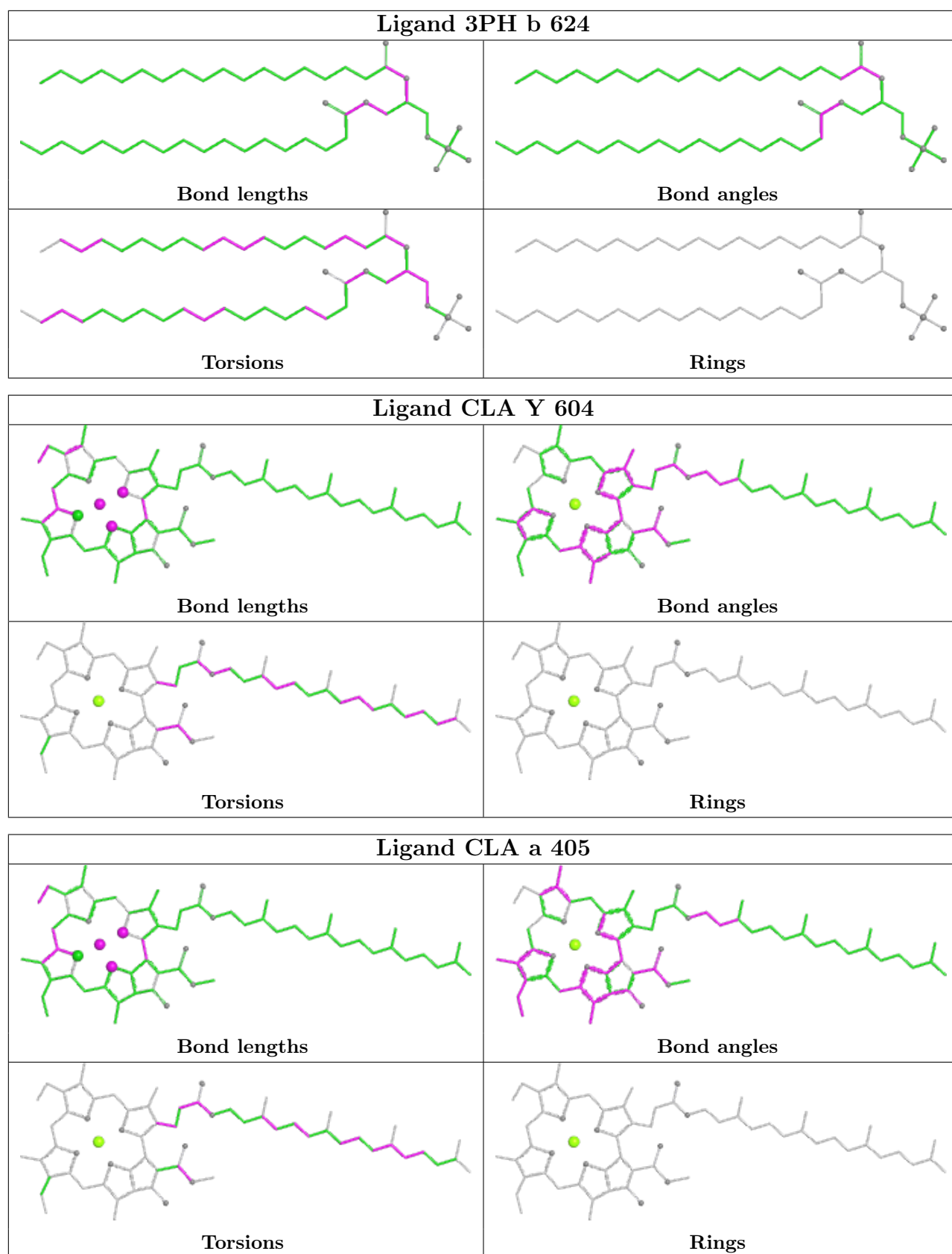


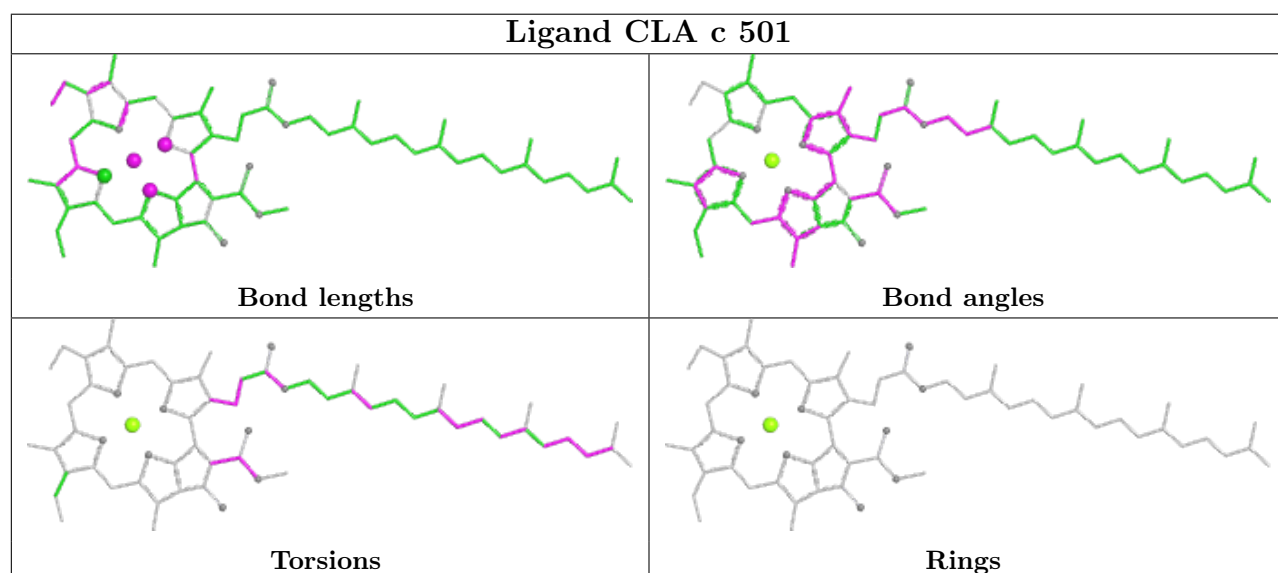
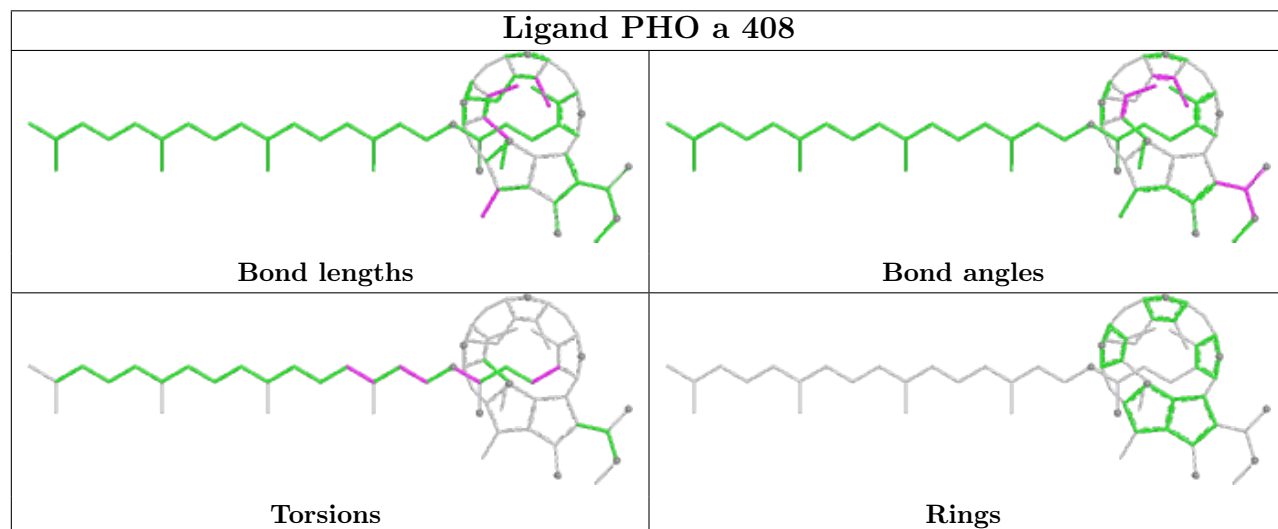
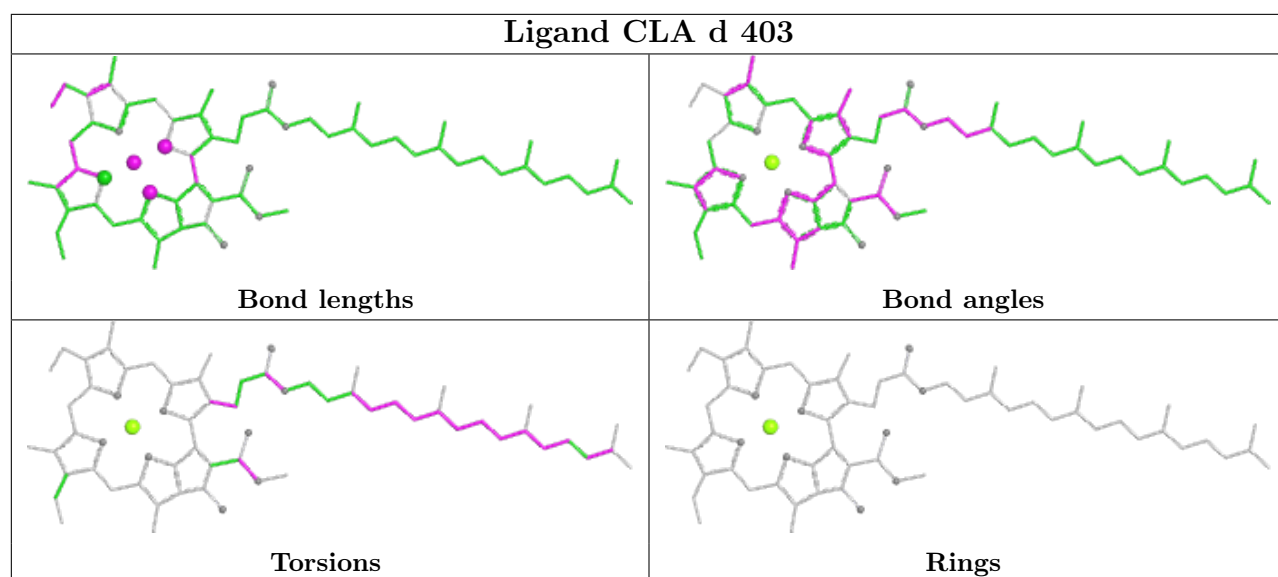
Ligand C7Z B 620

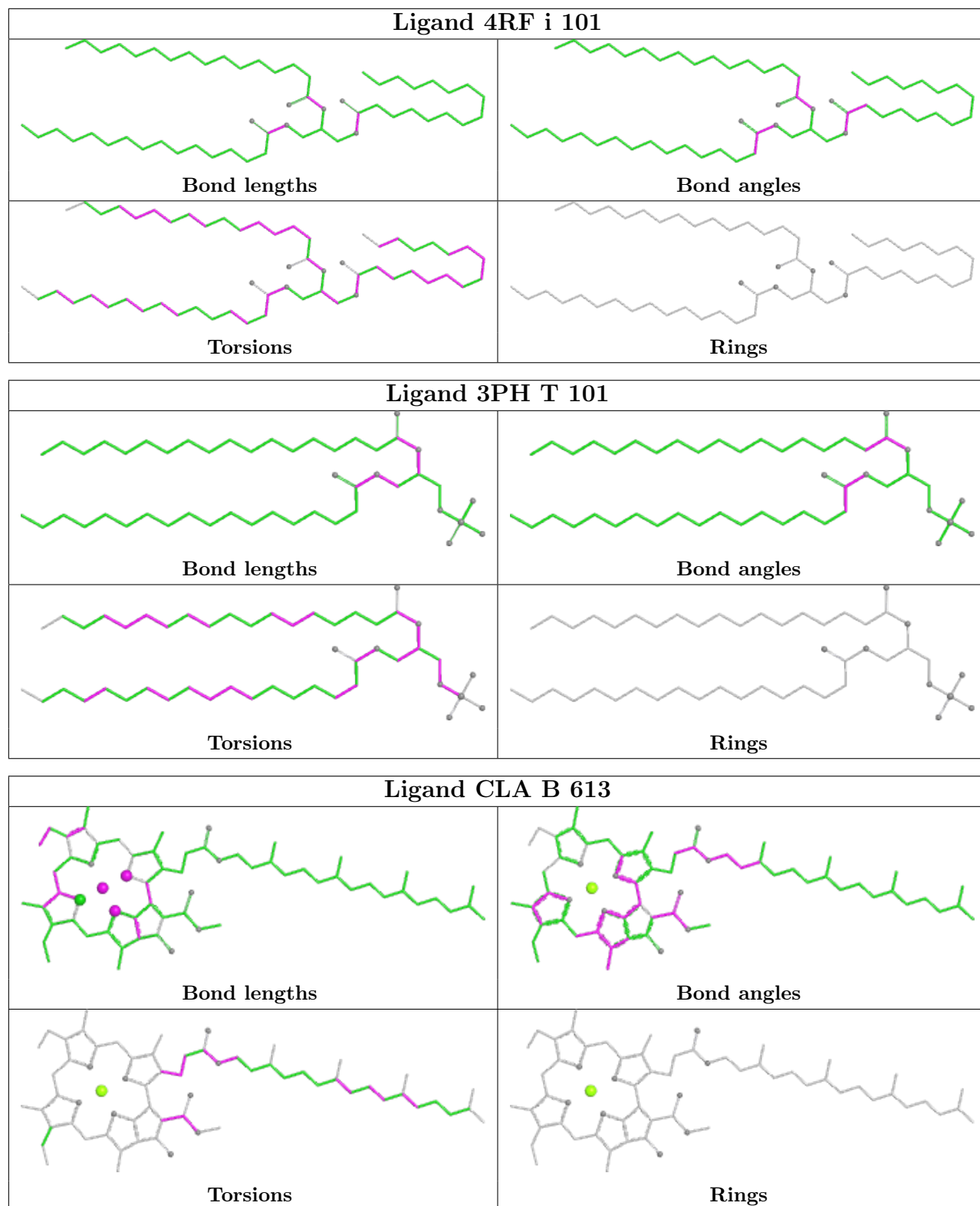


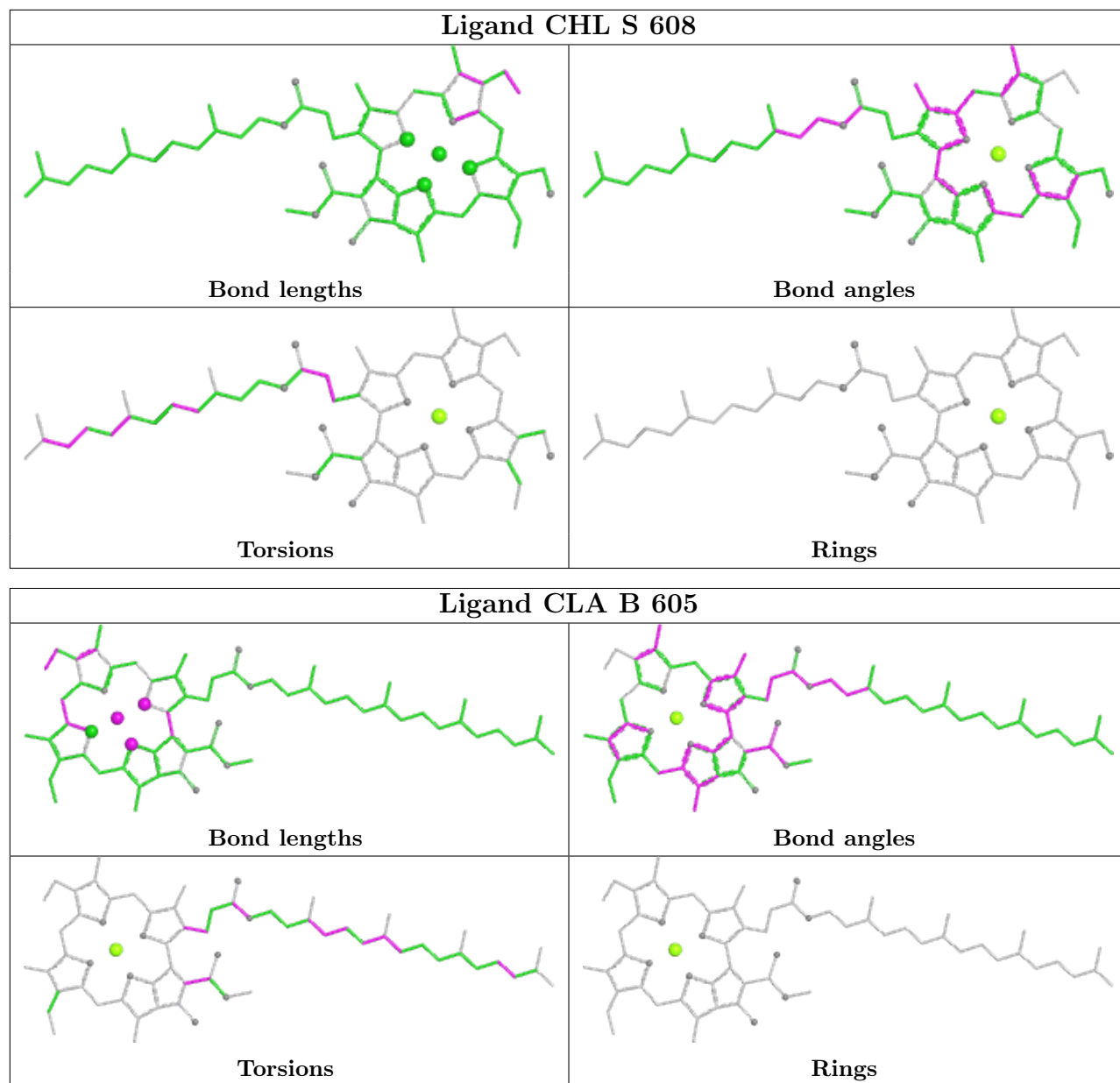
Ligand BCR C 515

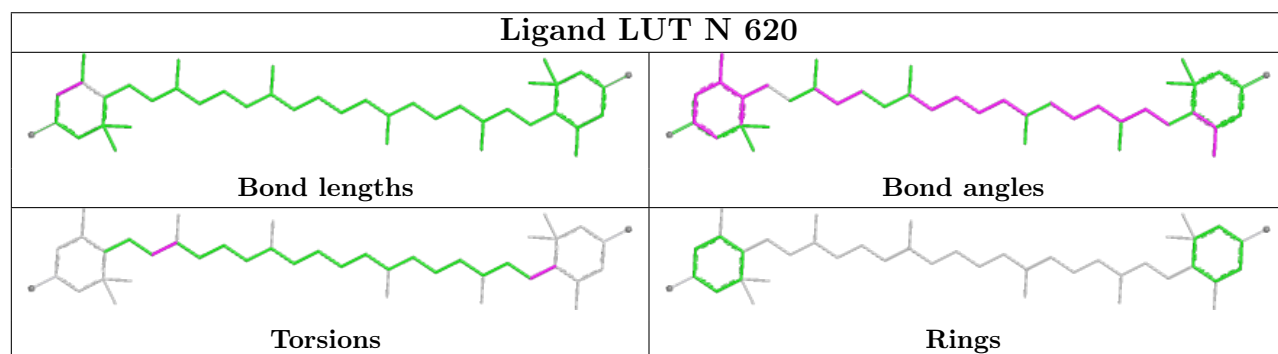
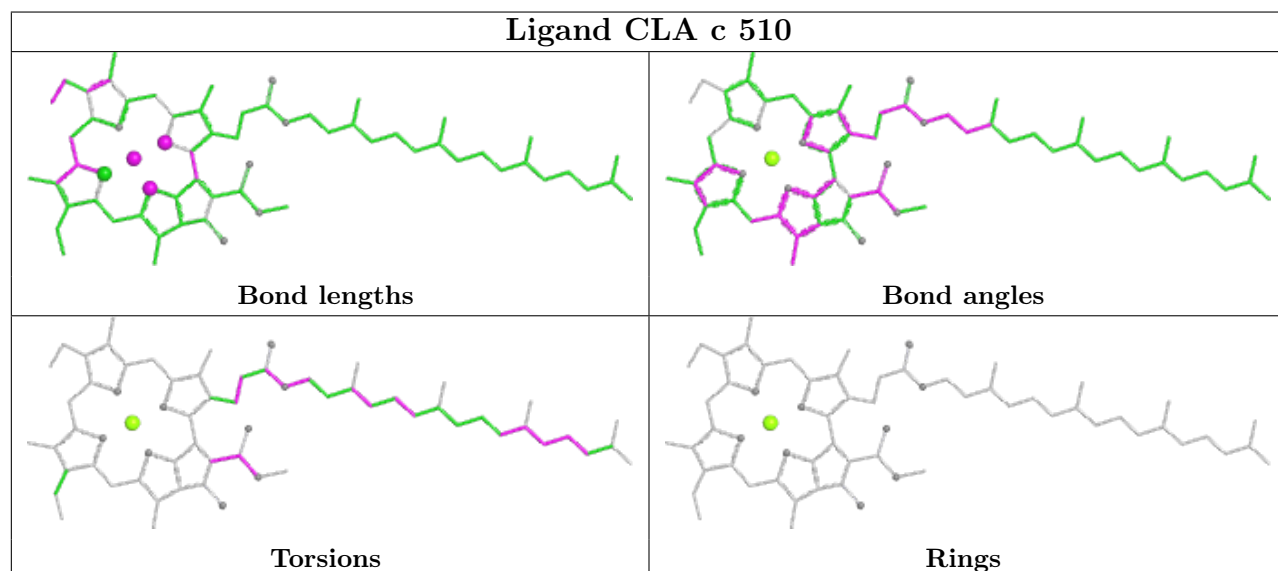
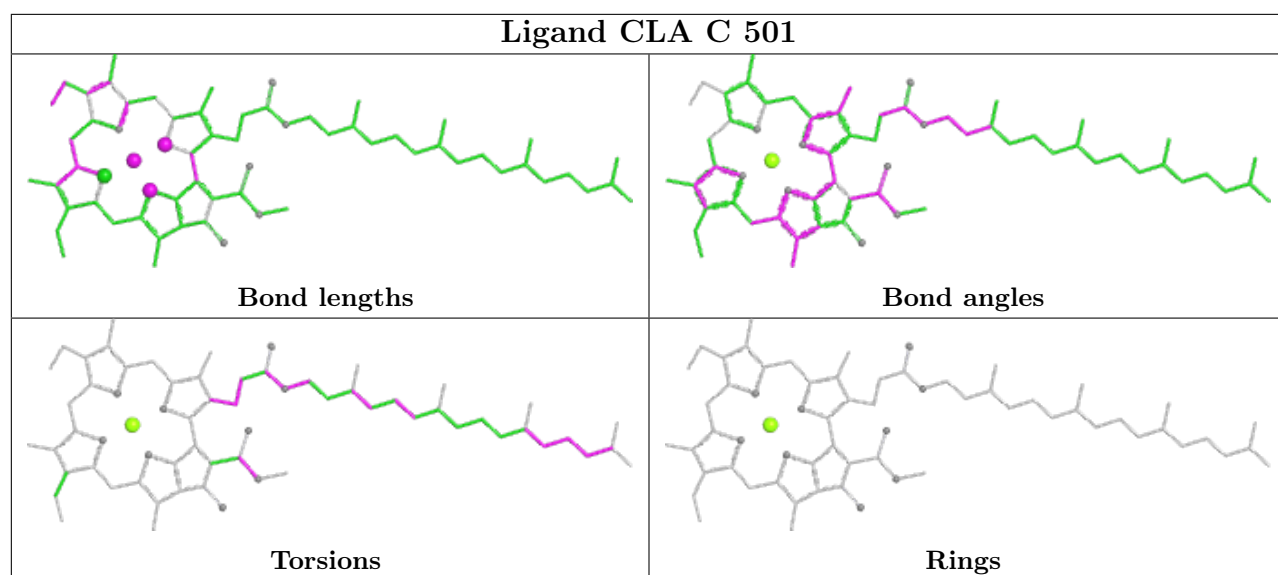


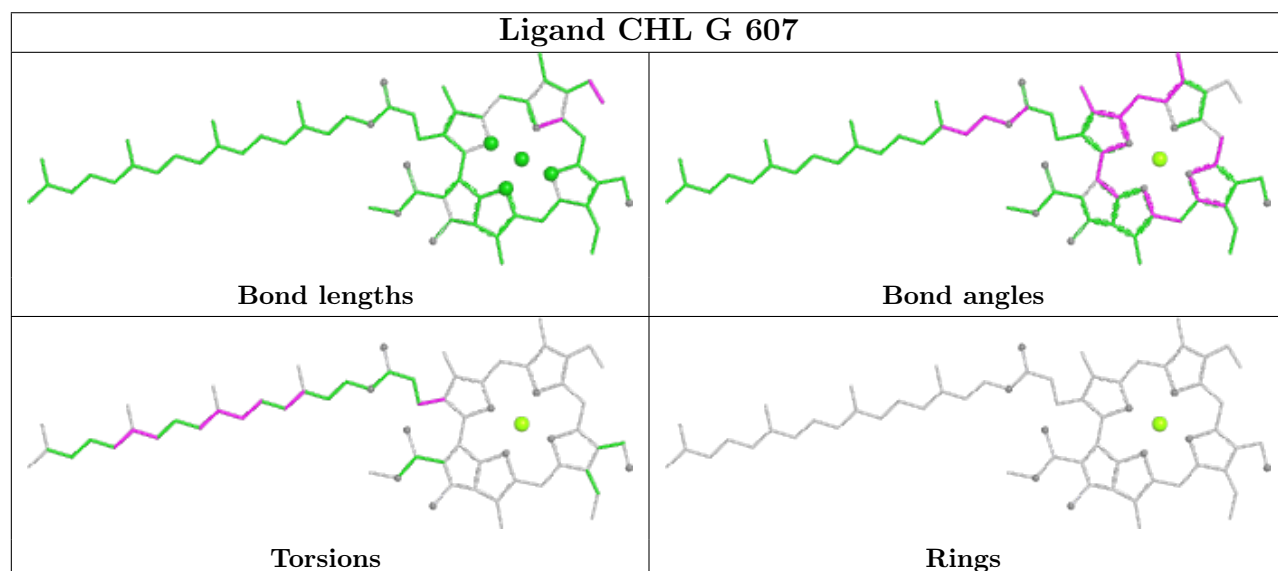
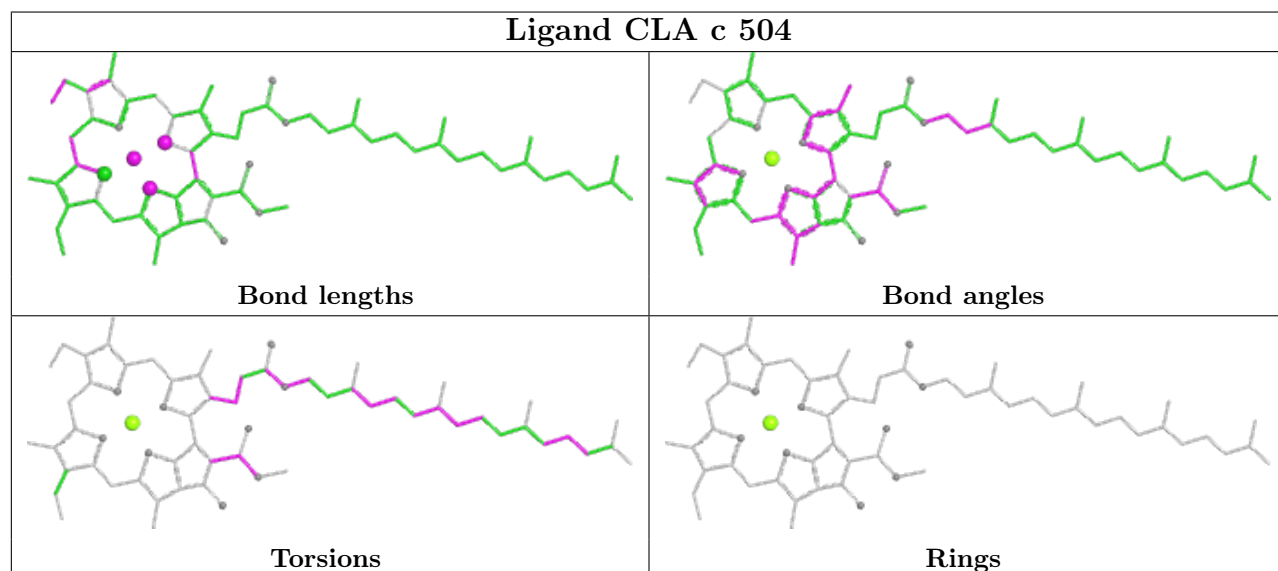
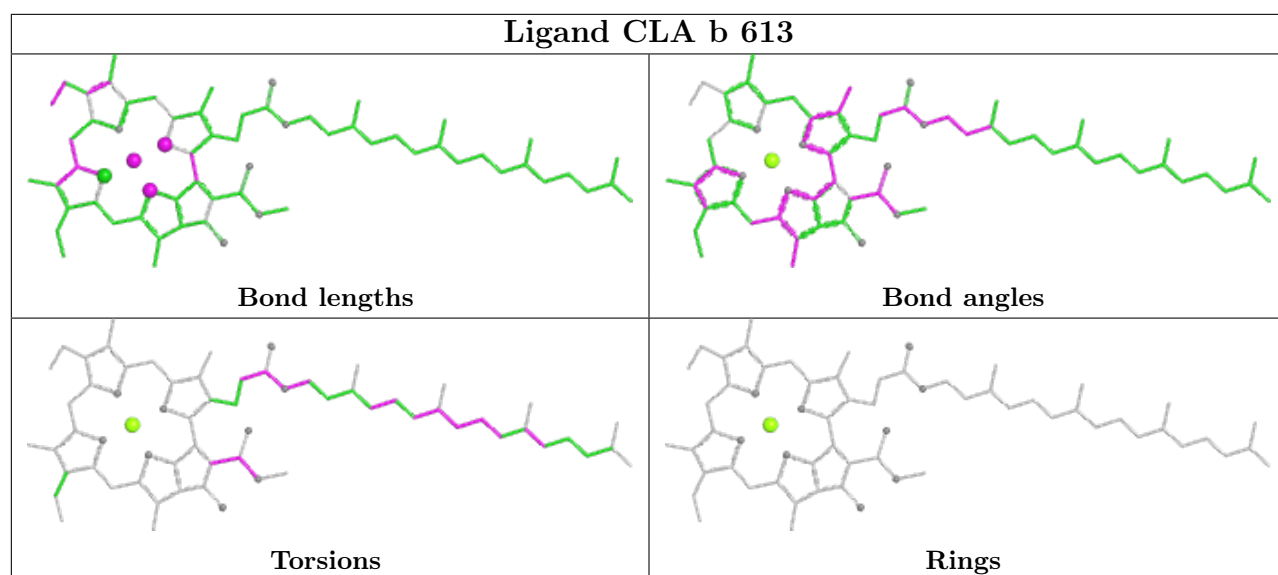


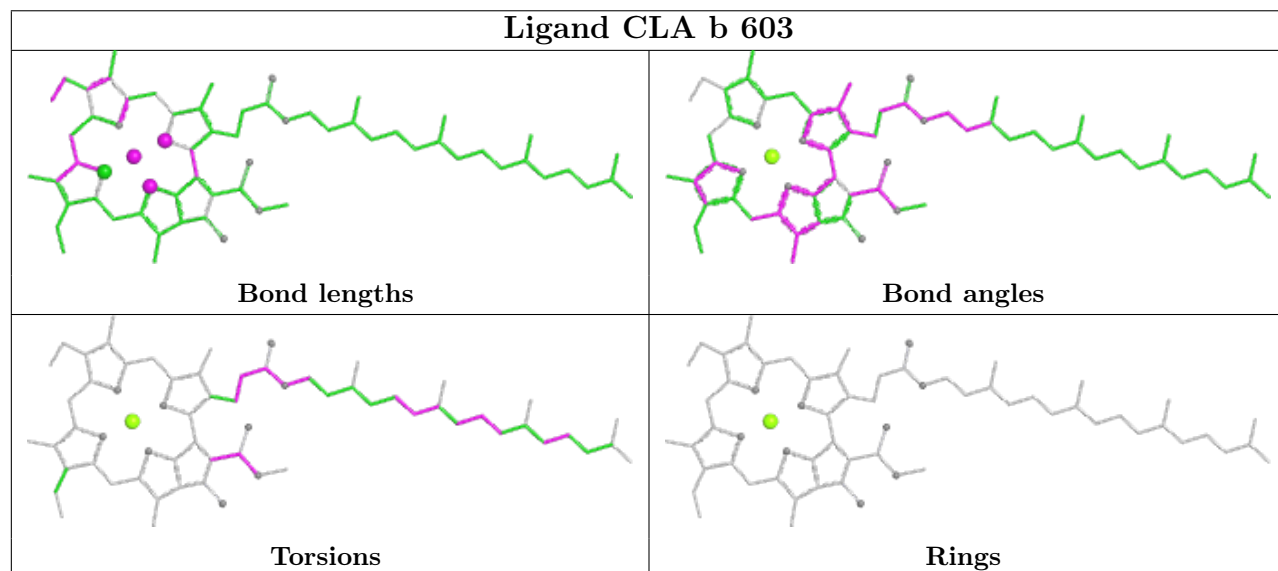
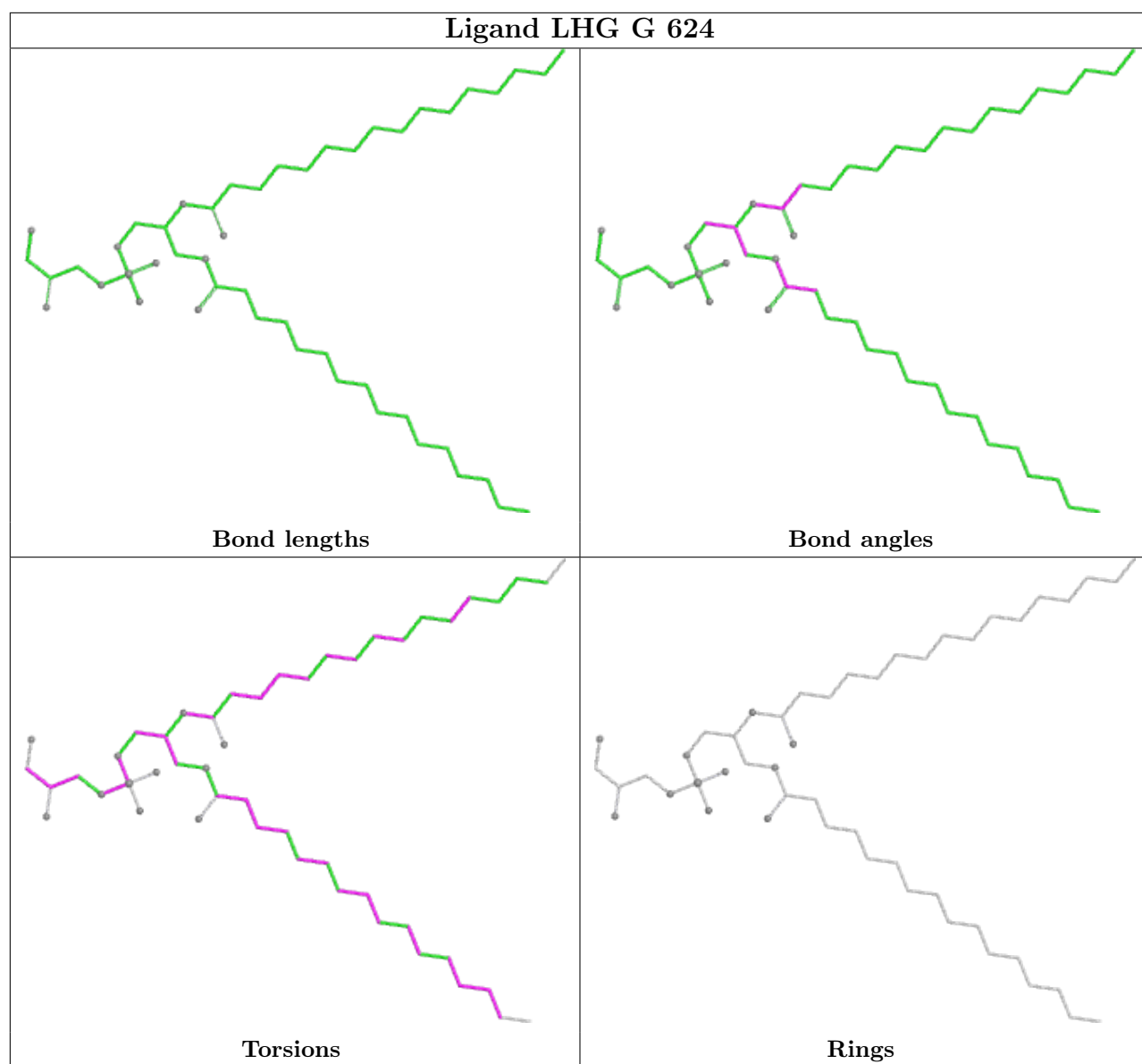


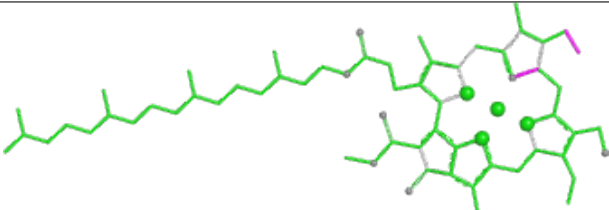
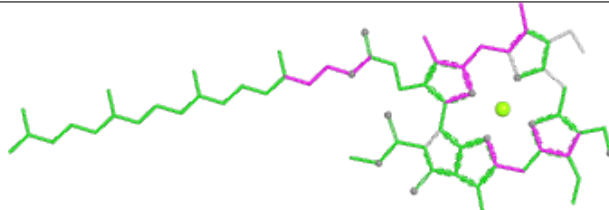
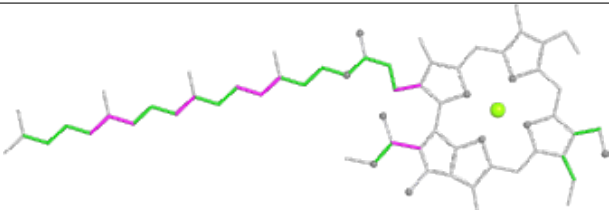
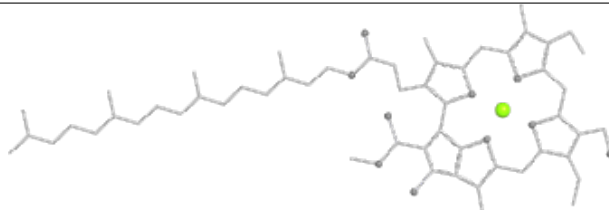


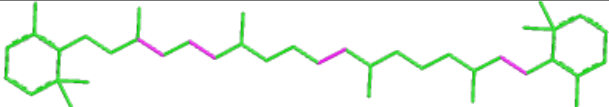
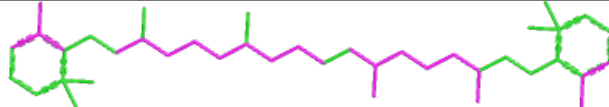
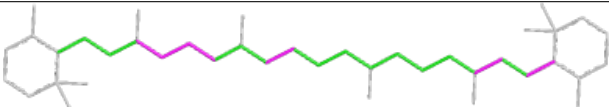
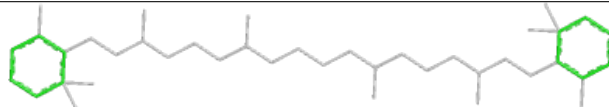


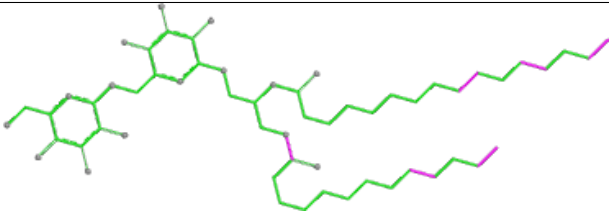
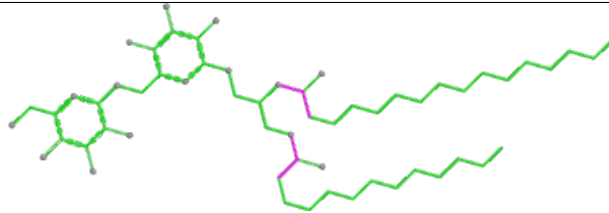
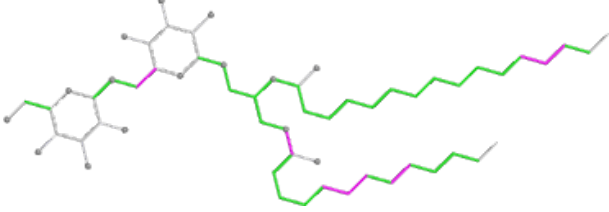
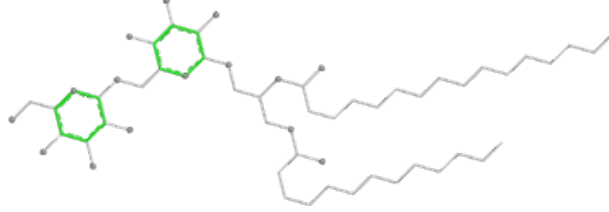


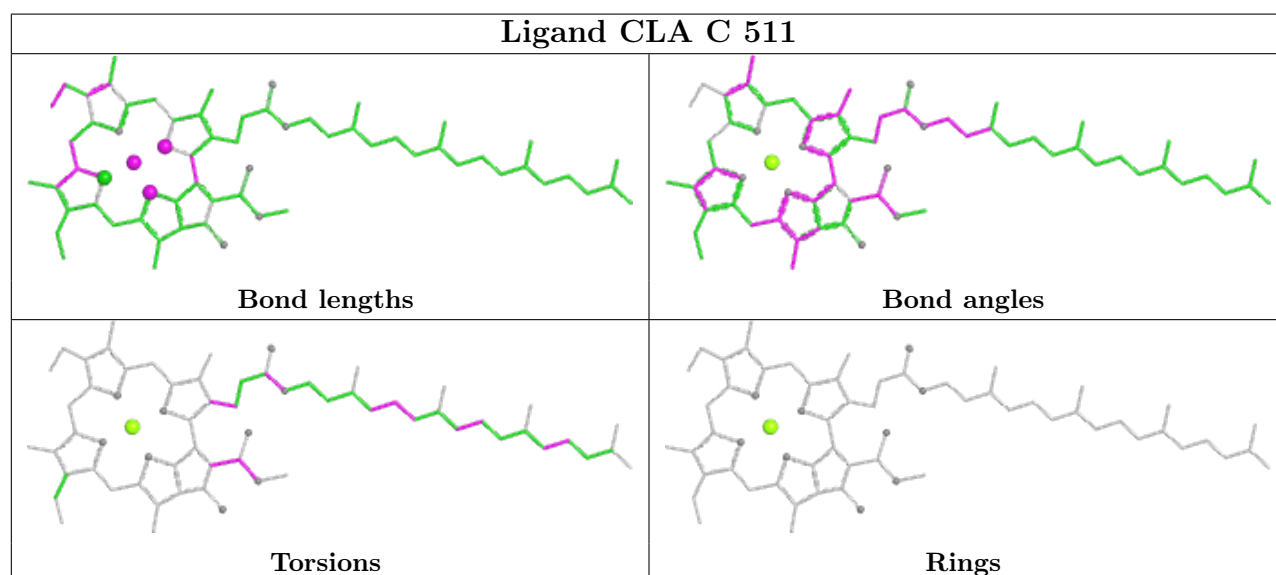
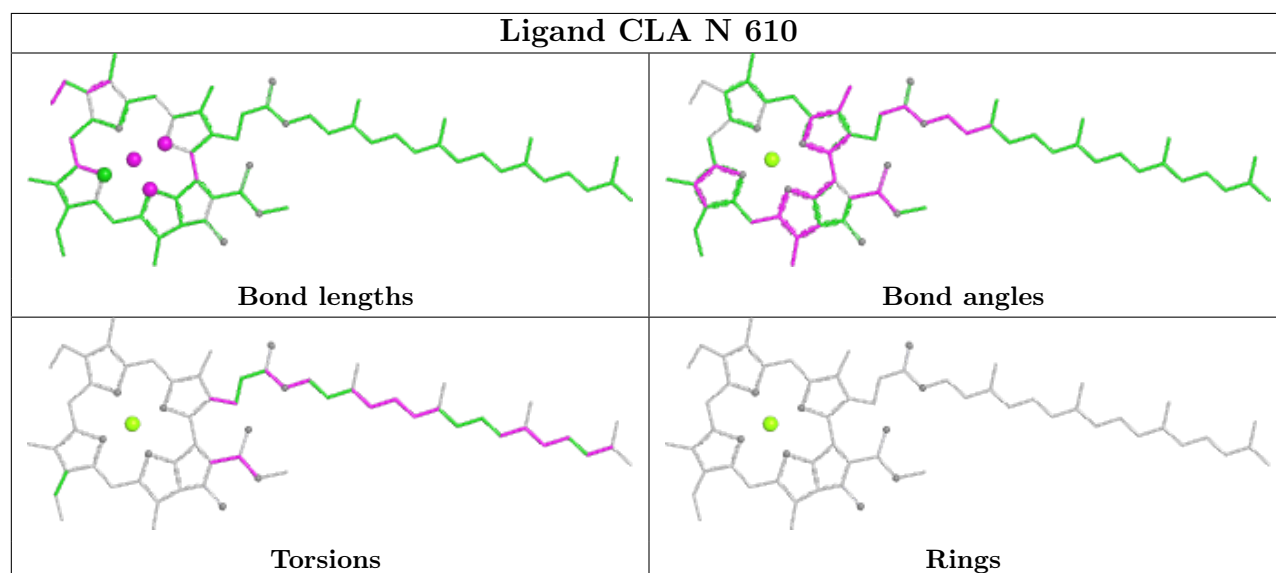
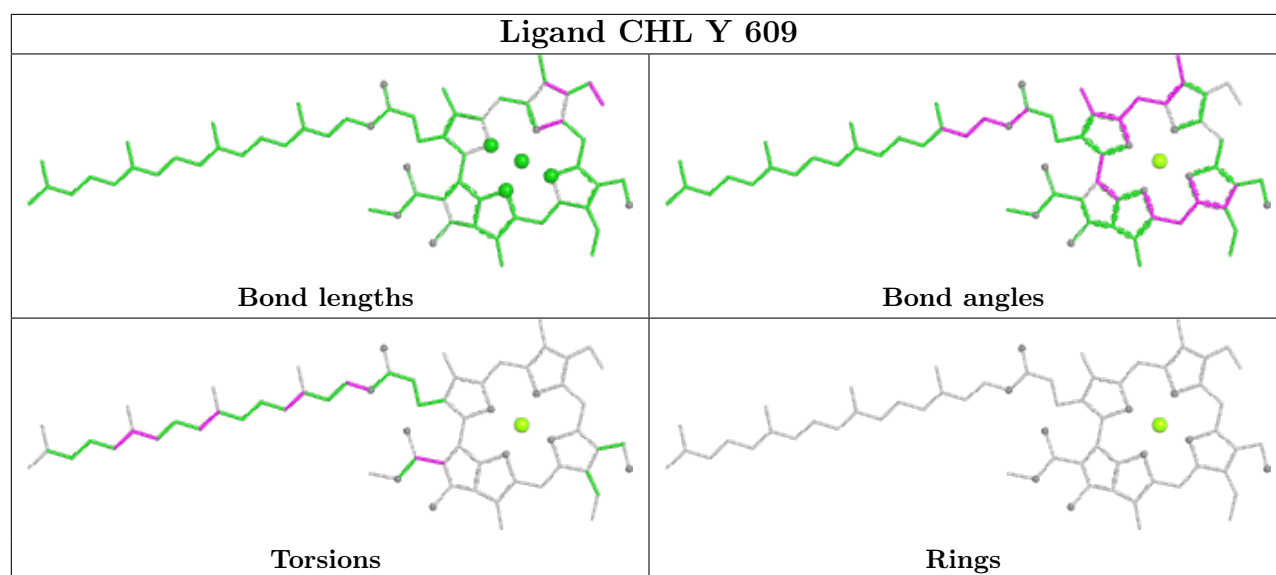


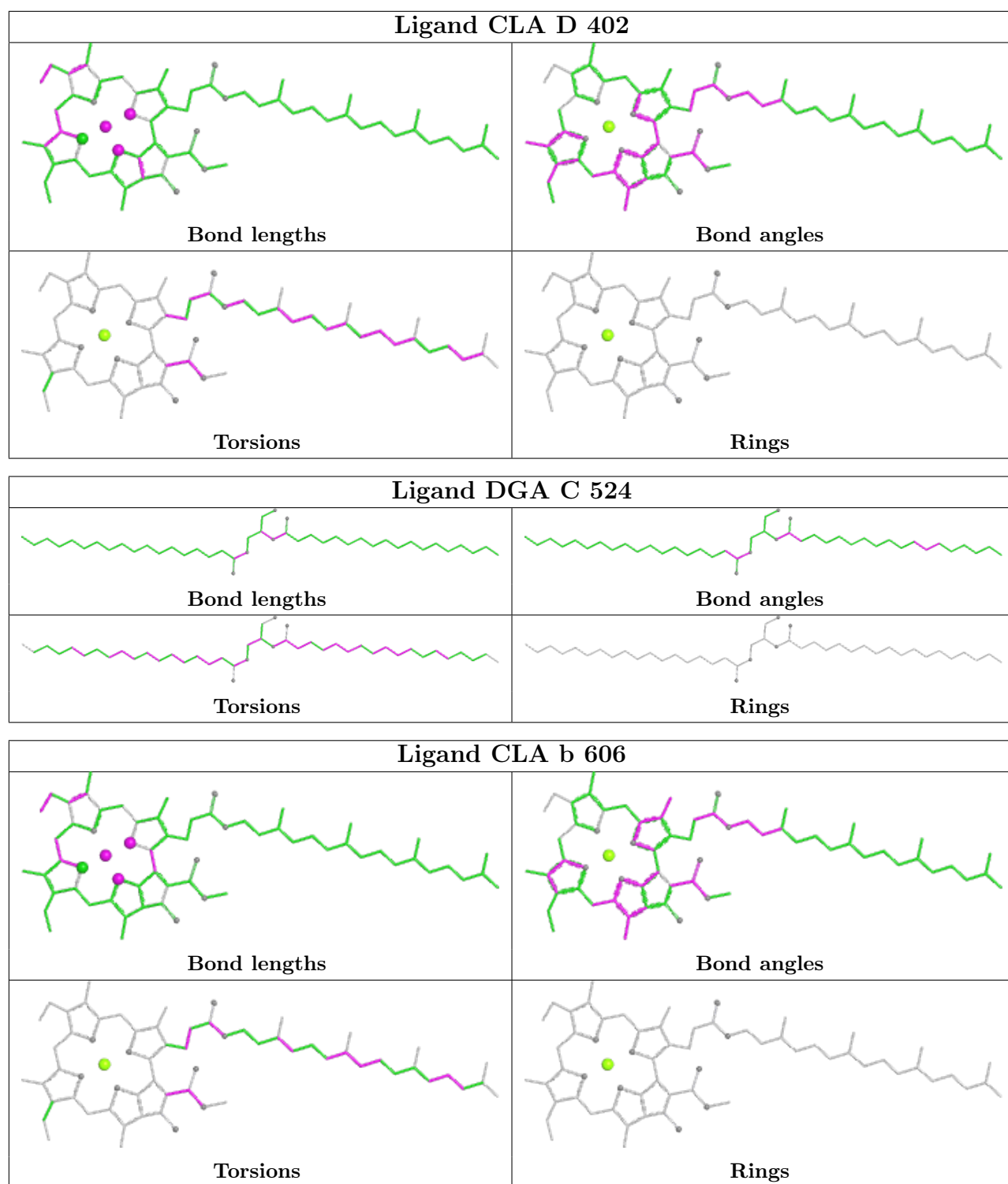


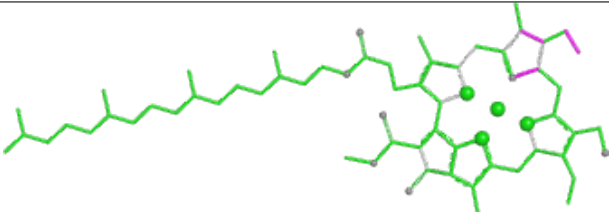
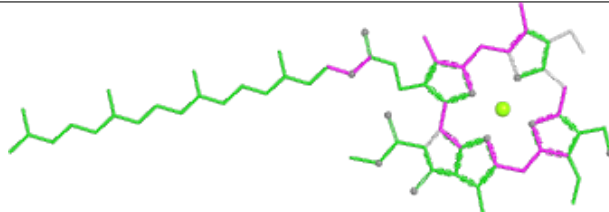
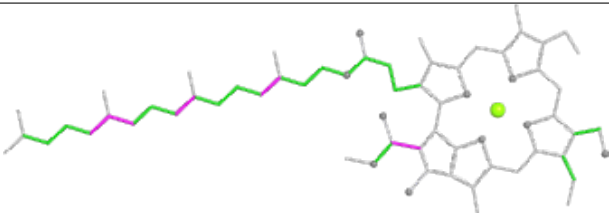
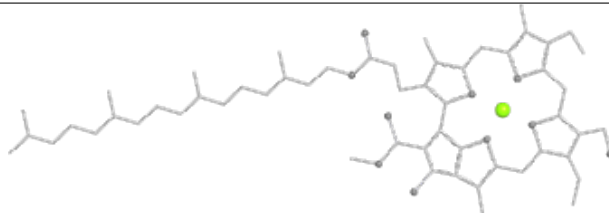
Ligand CHL N 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

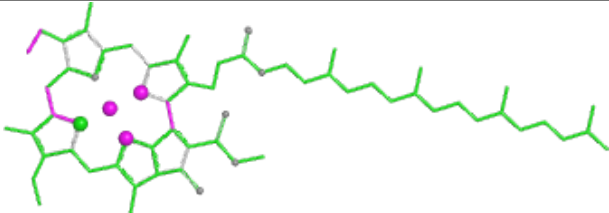
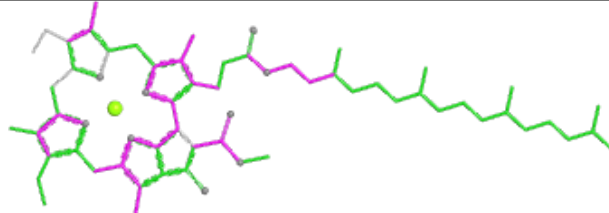
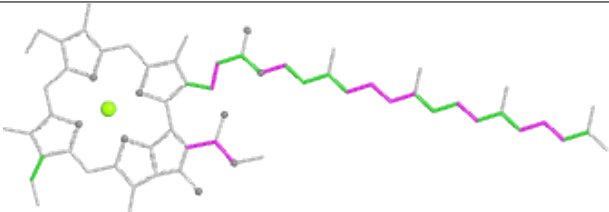
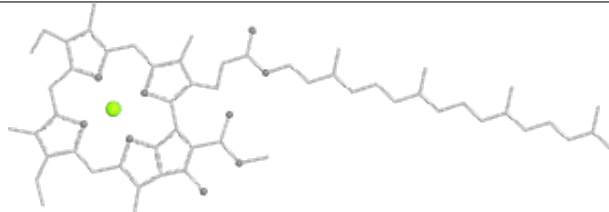
Ligand BCR c 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

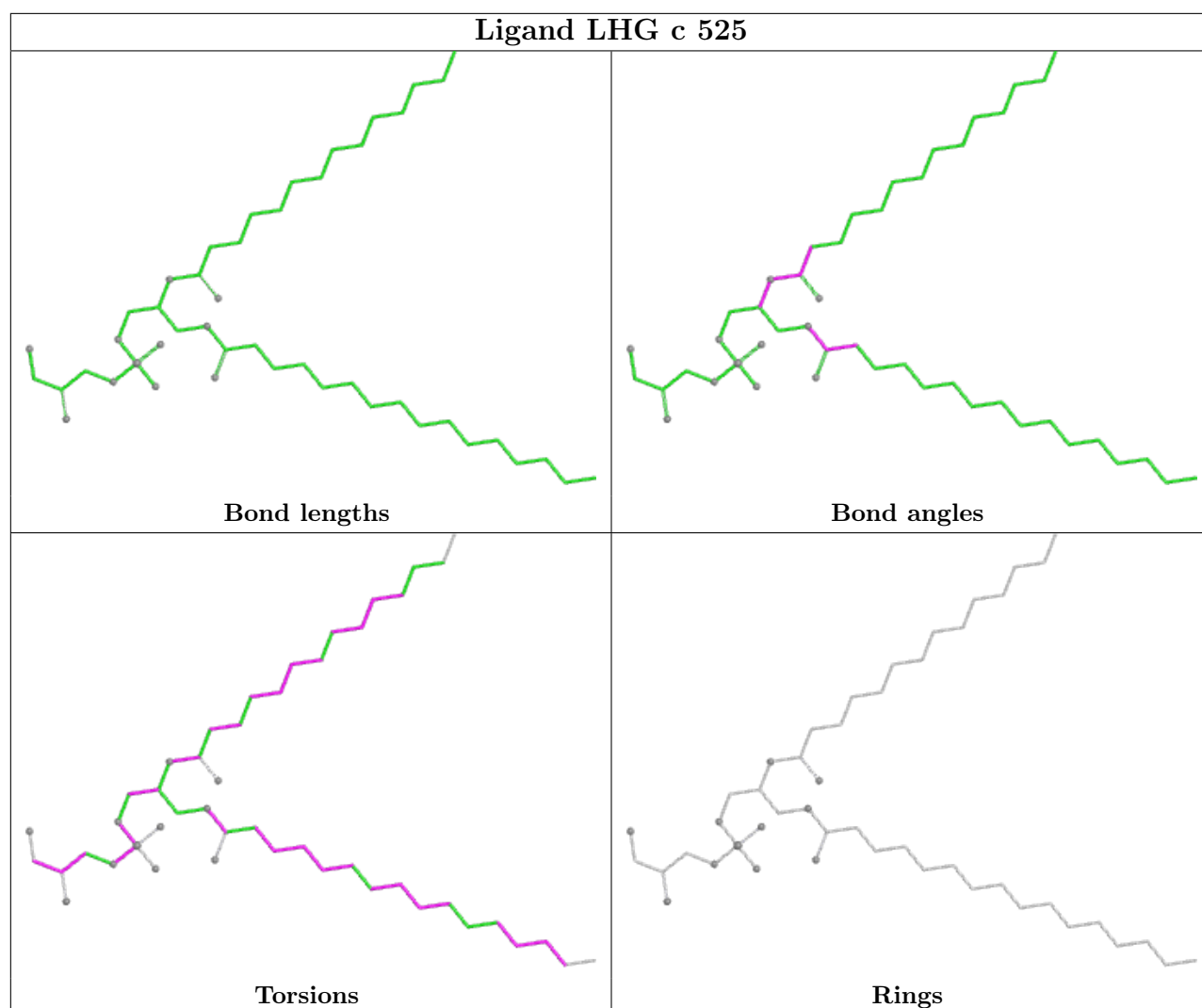
Ligand DGD C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings





Ligand CHL G 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13548. These allow visual inspection of the internal detail of the map and identification of artifacts.

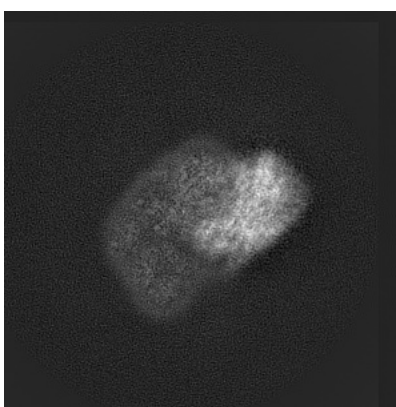
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

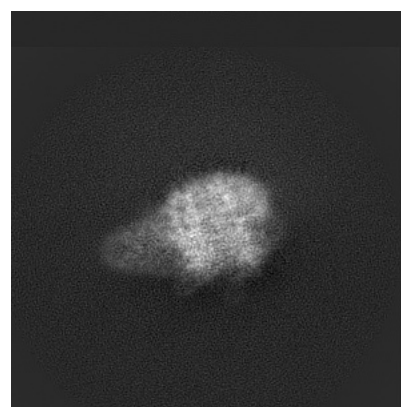
6.1.1 Primary map



X



Y

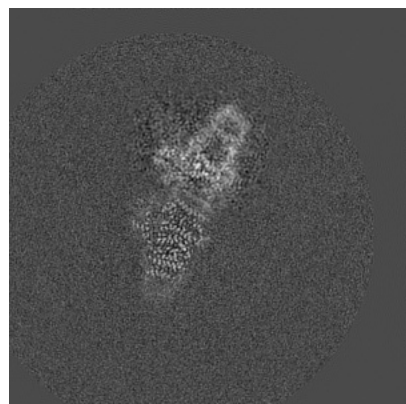


Z

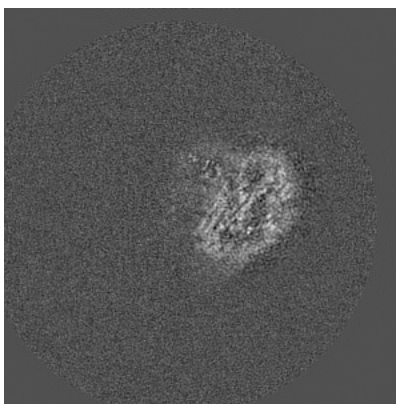
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

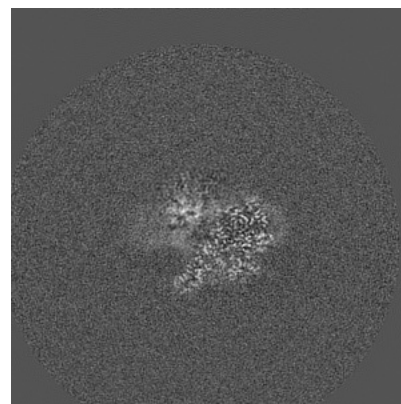
6.2.1 Primary map



X Index: 250



Y Index: 250

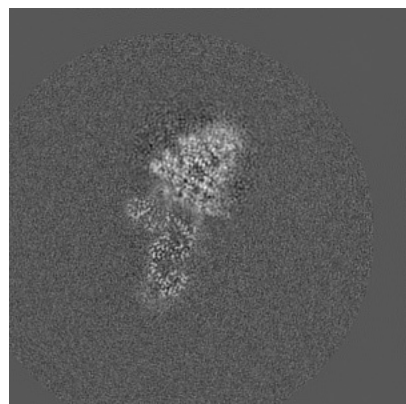


Z Index: 250

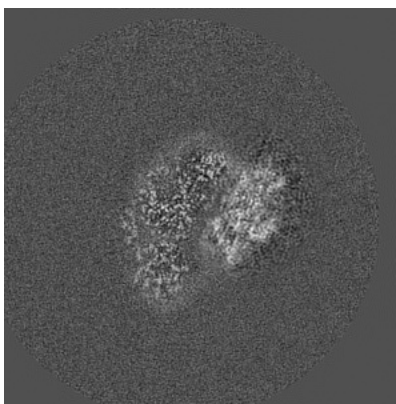
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

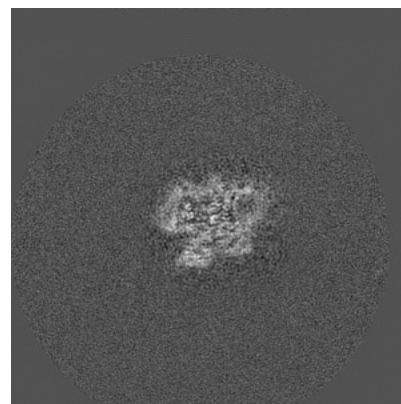
6.3.1 Primary map



X Index: 225



Y Index: 219



Z Index: 304

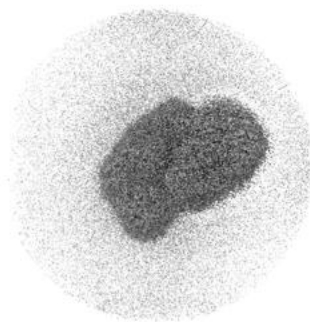
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

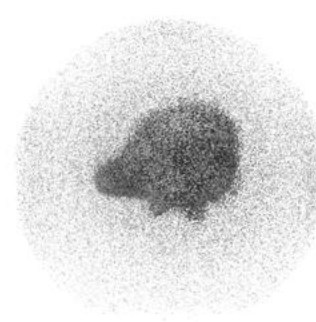
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

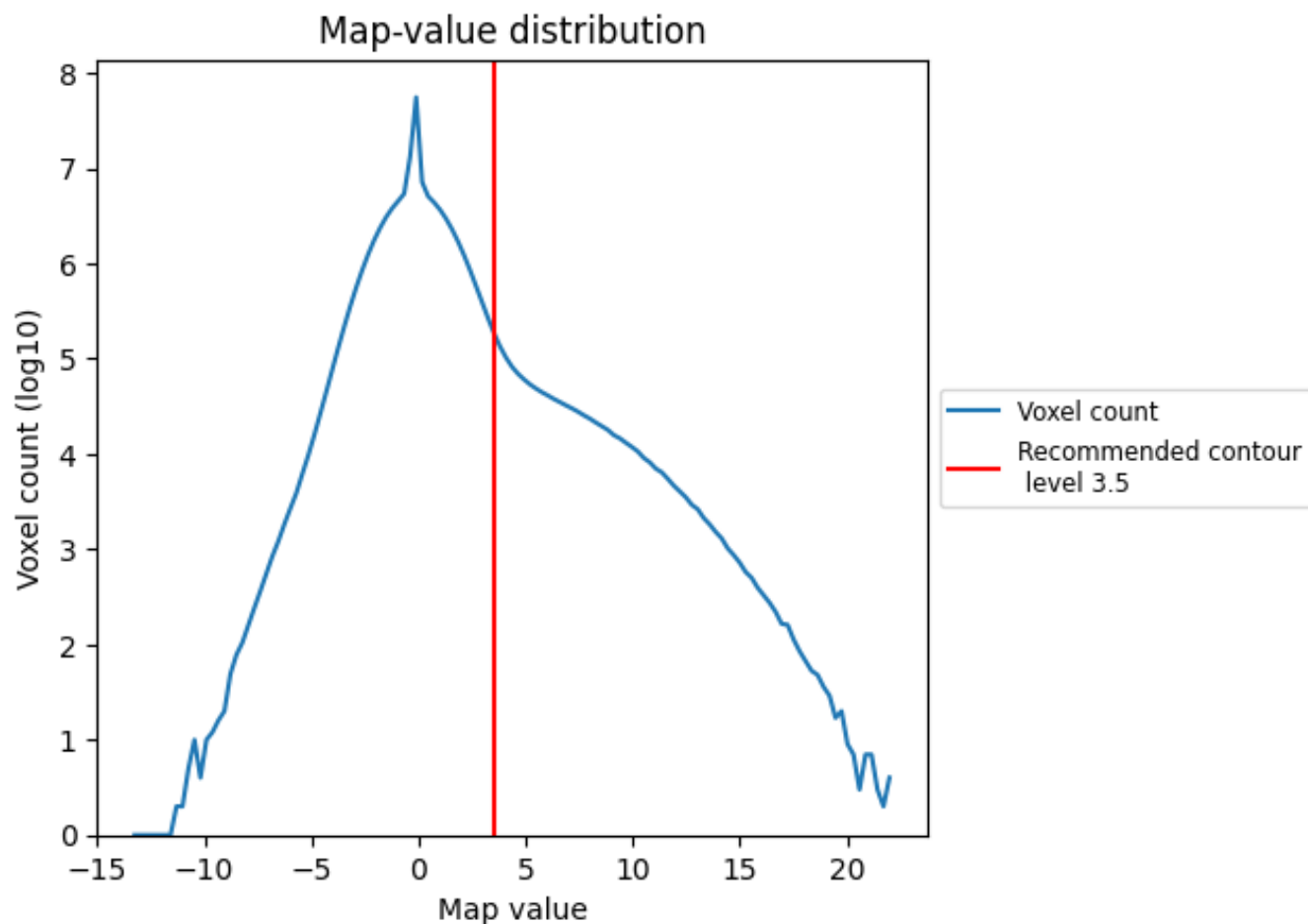
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

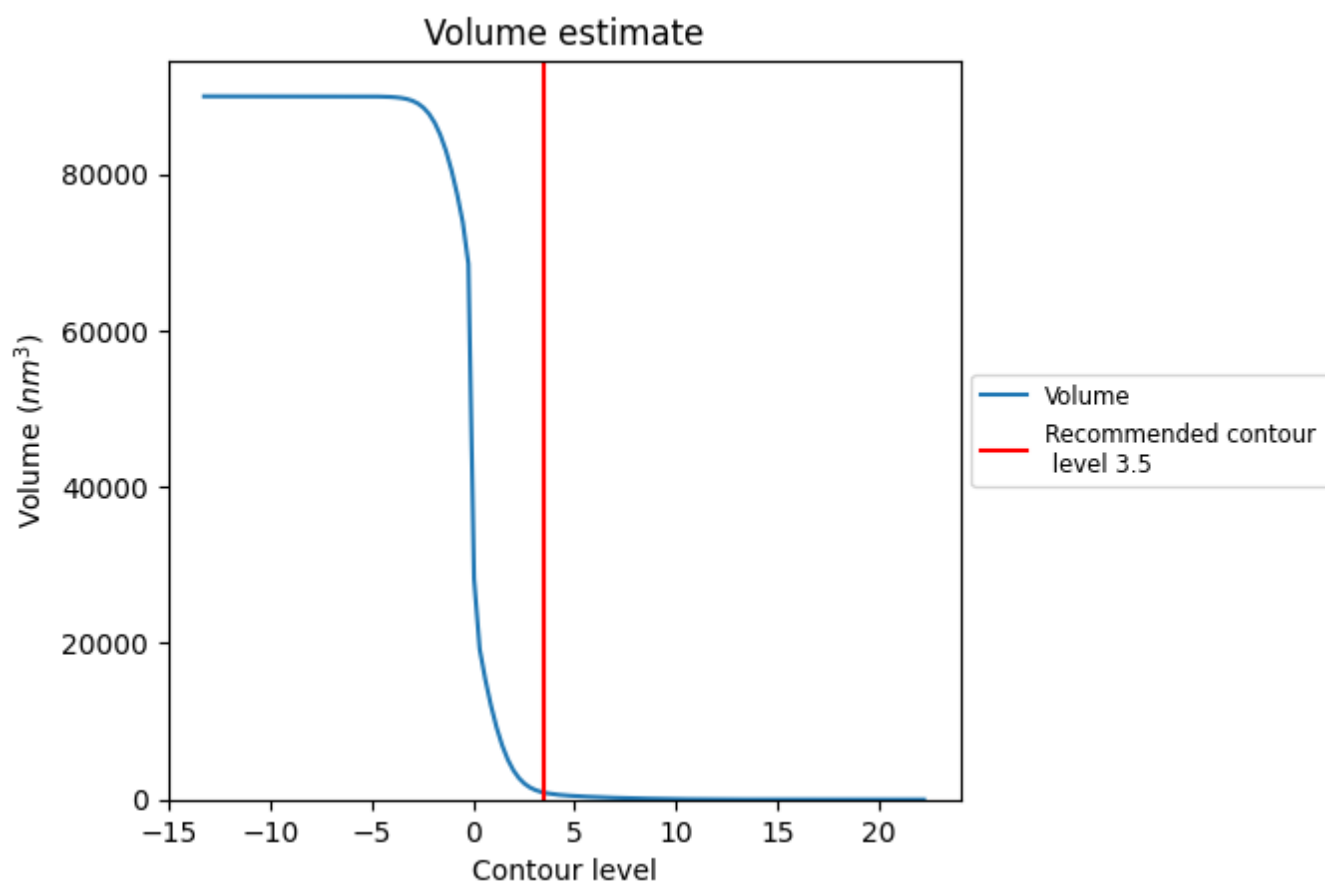
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

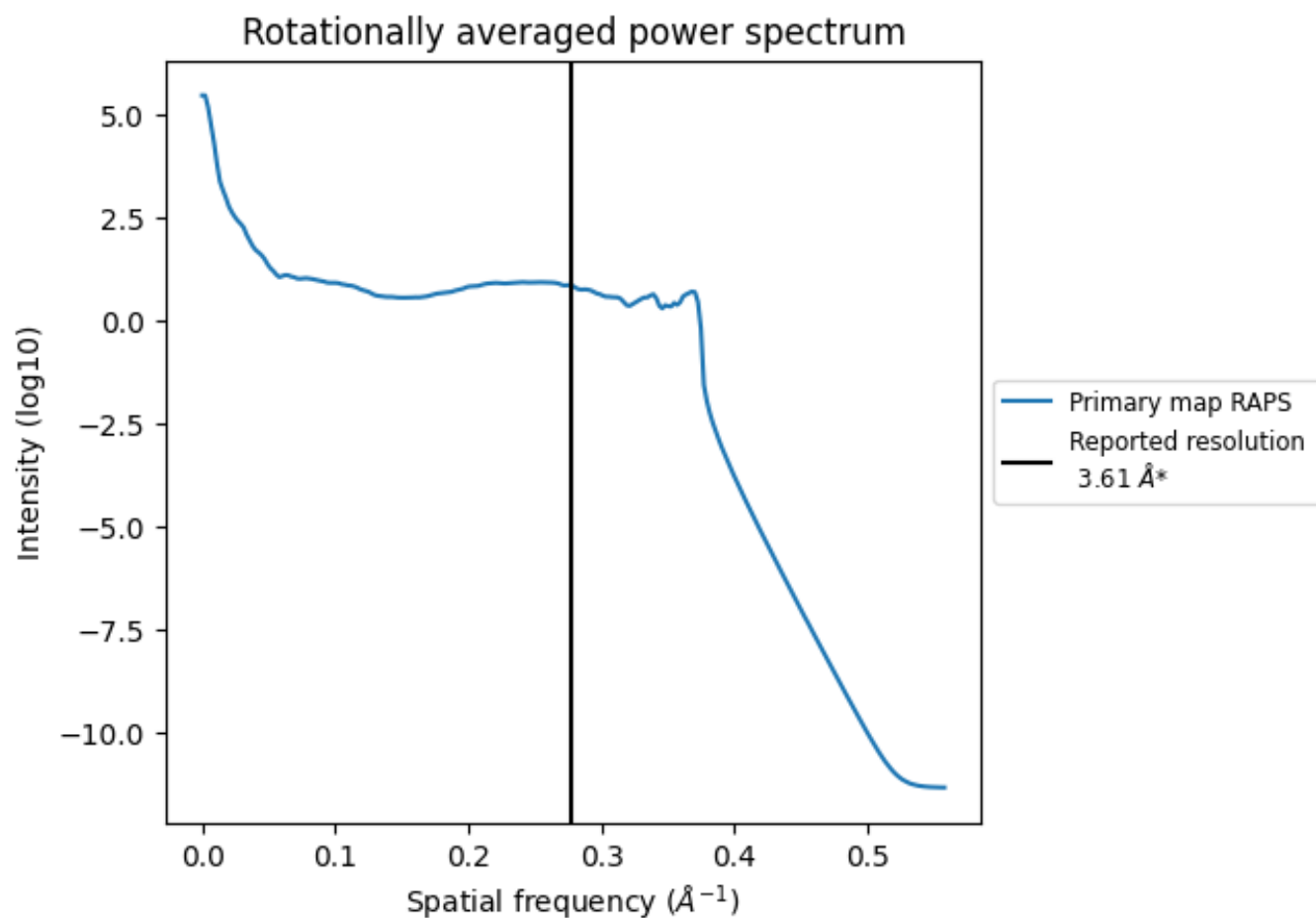
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 898 nm³; this corresponds to an approximate mass of 811 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

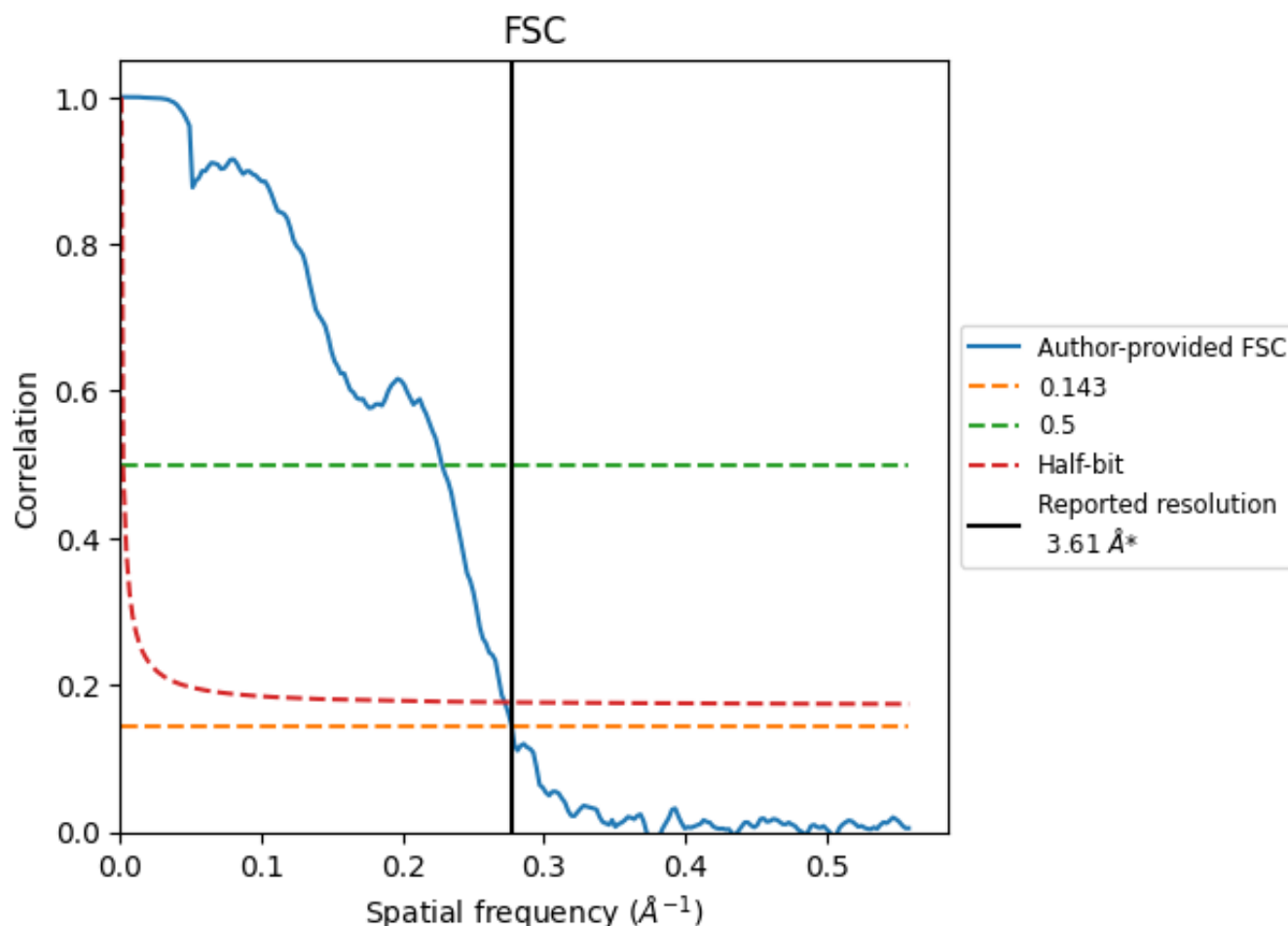


*Reported resolution corresponds to spatial frequency of 0.277 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.277 \AA^{-1}

8.2 Resolution estimates [i](#)

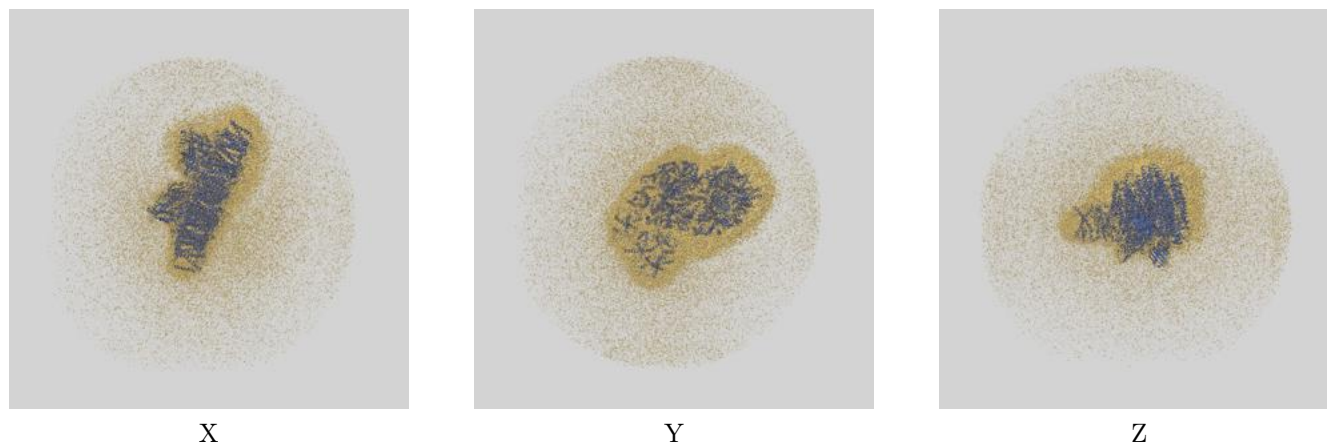
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.61	-	-
Author-provided FSC curve	3.61	4.39	3.67
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

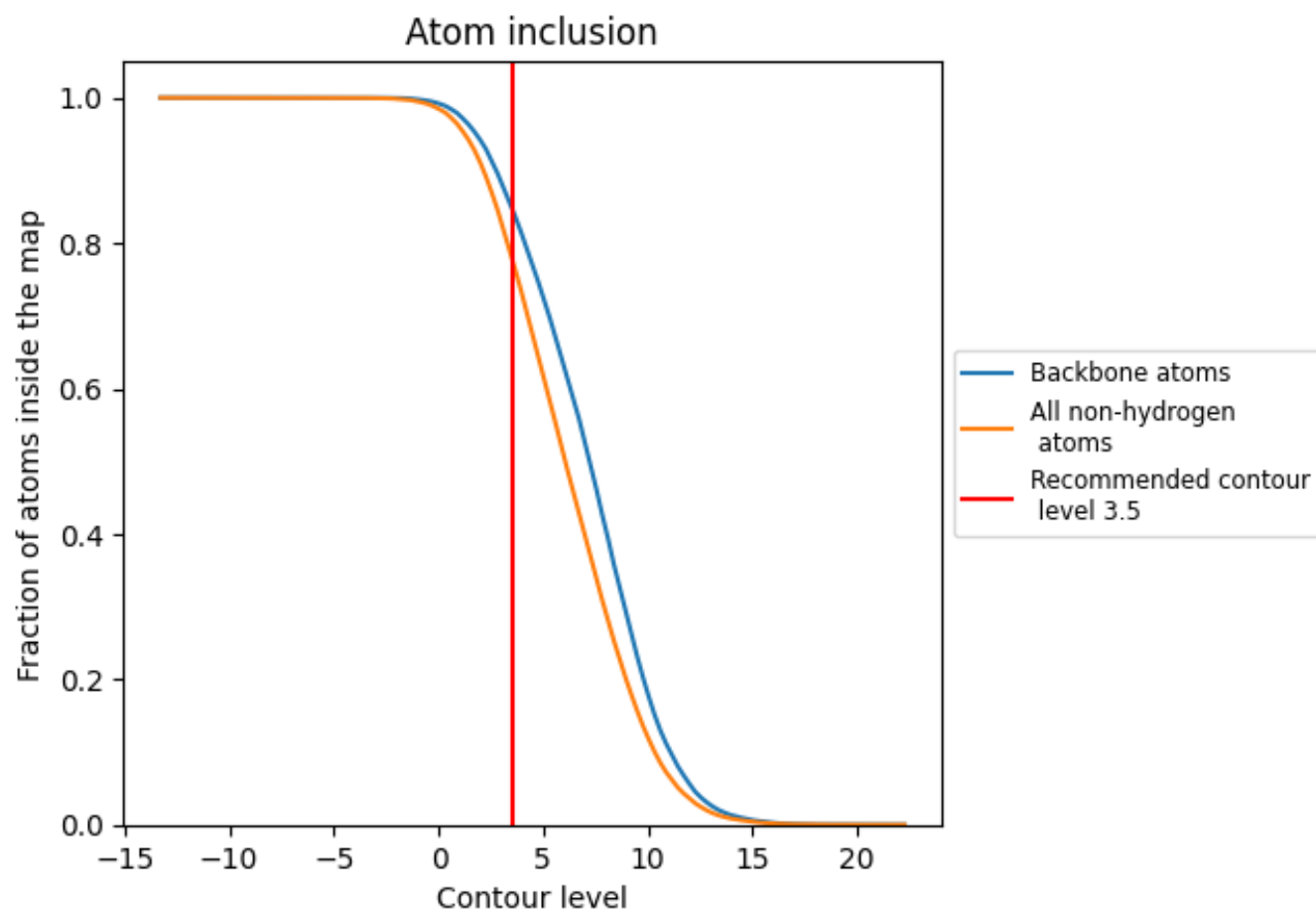
This section contains information regarding the fit between EMDB map EMD-13548 and PDB model 7PNK. Per-residue inclusion information can be found in section [3](#) on page [37](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.